Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	9VR0 / pdb_00009vr0
BMRB ID	:	36771
Title	:	NMR solution structure of termini-truncated oxidized cytochrome c552 from Thioalkalivibrio paradoxus
Authors	:	Britikov, V.V.; Britikova, E.V.; Rakitina, T.V.; Dergousova, N.I.; Tikhonova, T.V.; Popov, V.O.; Bocharov, E.V.
Deposited on	:	2025-07-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

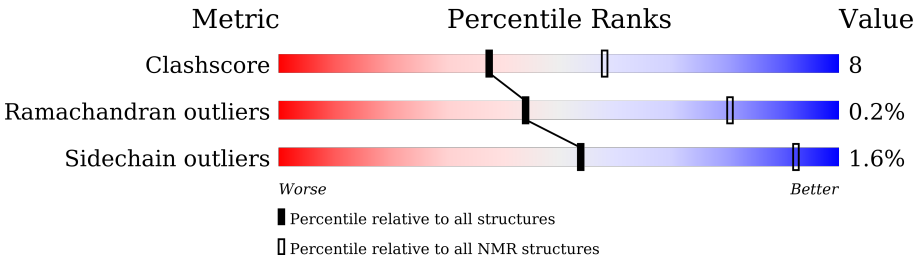
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	125	78% 6% 9% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	HEC	201	20	-

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:26-A:130 (105)	0.65	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 18, 19
2	4, 9, 15, 17, 20
Single-model clusters	10; 16

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1773 atoms, of which 847 are hydrogens and 0 are deuteriums.

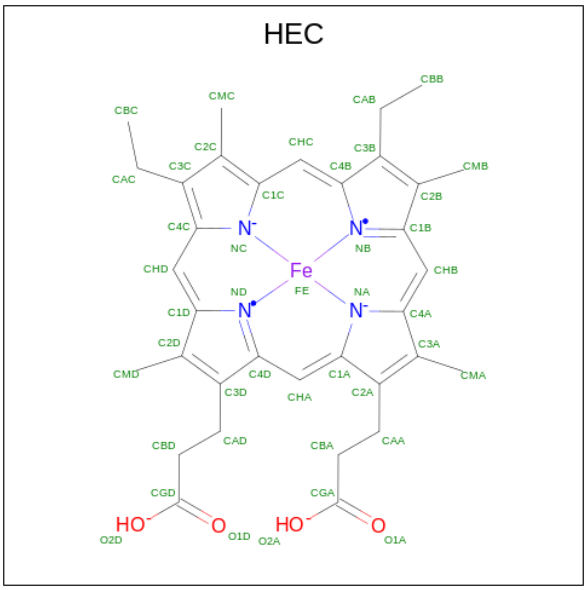
- Molecule 1 is a protein called Cytochrome c552.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	116	1698	540	815	167	172	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A8J0PCM1
A	137	LEU	-	expression tag	UNP A0A8J0PCM1
A	138	GLU	-	expression tag	UNP A0A8J0PCM1
A	139	HIS	-	expression tag	UNP A0A8J0PCM1
A	140	HIS	-	expression tag	UNP A0A8J0PCM1
A	141	HIS	-	expression tag	UNP A0A8J0PCM1
A	142	HIS	-	expression tag	UNP A0A8J0PCM1
A	143	HIS	-	expression tag	UNP A0A8J0PCM1
A	144	HIS	-	expression tag	UNP A0A8J0PCM1

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Cytochrome c552

Chain A:

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

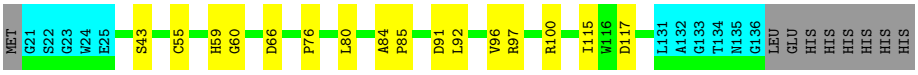
• Molecule 1: Cytochrome c552

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: Cytochrome c552

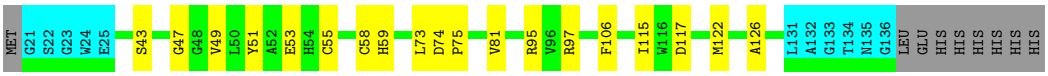
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c552

Chain A: 69% 15% 9% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c552

Chain A: 69% 15% 9% 7%

4.2.5 Score per residue for model 5

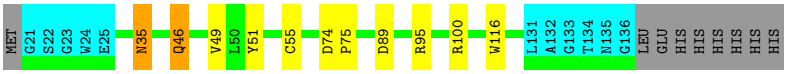
- Molecule 1: Cytochrome c552

Chain A: 74% 9% • 9% 7%

4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c552

Chain A: 75% 7% • 9% 7%



4.2.7 Score per residue for model 7

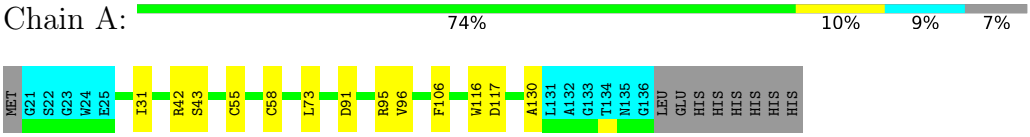
- Molecule 1: Cytochrome c552

Chain A: 69% 15% 9% 7%

4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c552

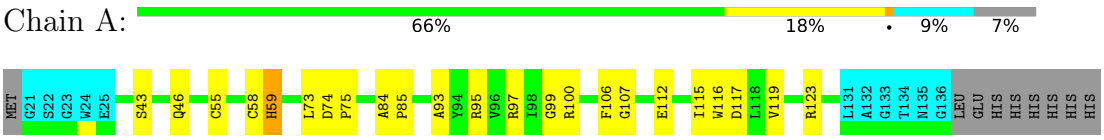
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c552

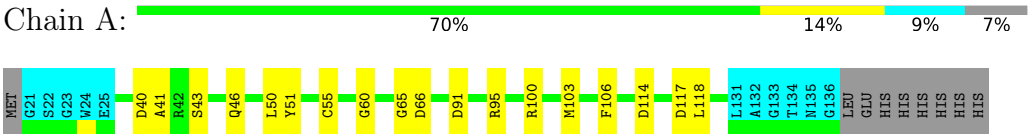
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c552

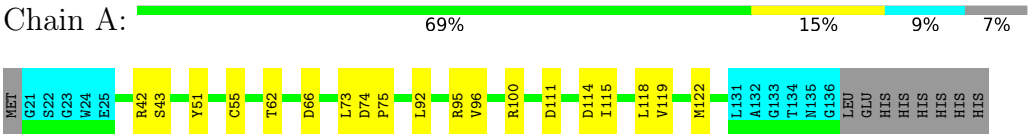
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c552

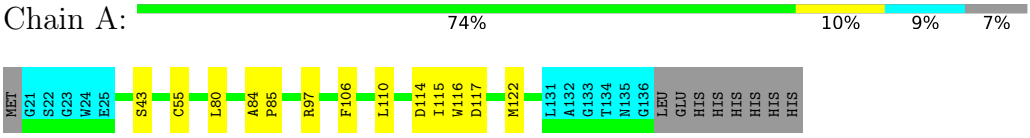
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c552

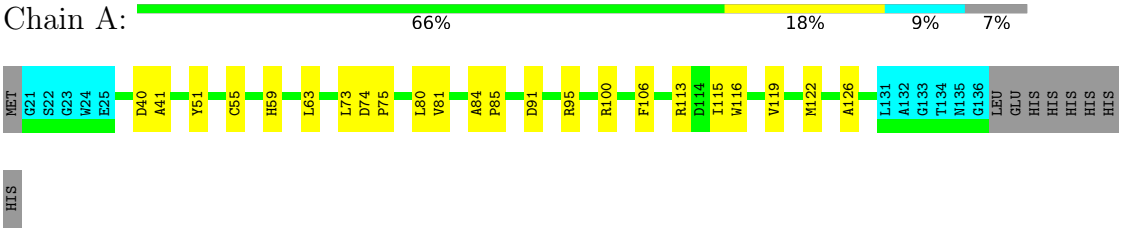
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c552

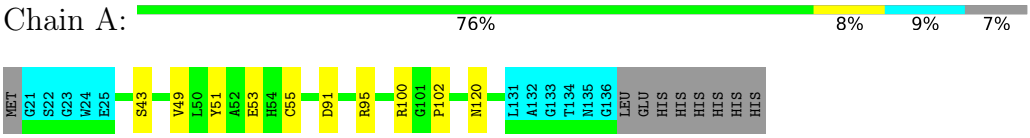
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c552

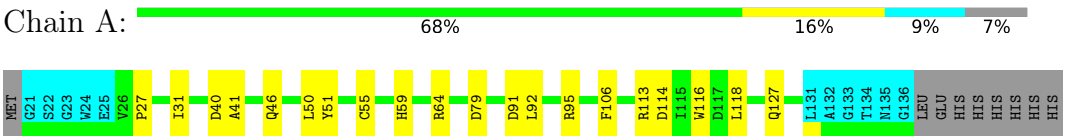
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome c552

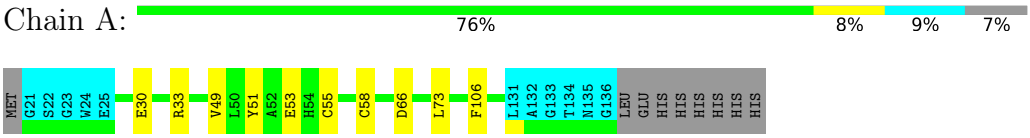
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c552

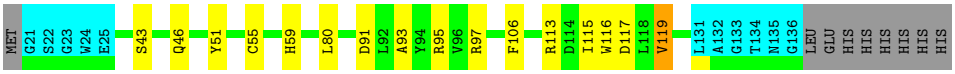
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome c552

Chain A:



4.2.18 Score per residue for model 18

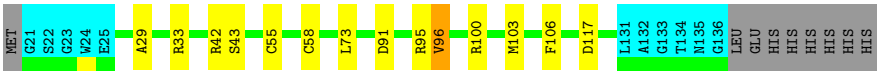
- Molecule 1: Cytochrome c552

Chain A:

4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c552

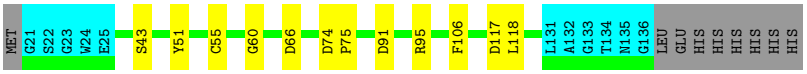
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c552

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 128 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	1.3
CNS	structure calculation	1.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1184
Number of shifts mapped to atoms	1184
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	810	753	747	11±3
2	A	43	32	30	5±2
All	All	17060	15700	15540	245

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:201:HEC:HBC3	2:A:201:HEC:HMC1	0.72	1.61	3	2
1:A:58:CYS:SG	1:A:73:LEU:HD11	0.68	2.28	8	6
1:A:122:MET:HE1	2:A:201:HEC:HMA2	0.67	1.65	13	3
2:A:201:HEC:HMC1	2:A:201:HEC:HBC3	0.66	1.66	9	1
2:A:201:HEC:HMC3	2:A:201:HEC:CBC	0.66	2.21	18	3
2:A:201:HEC:HMC3	2:A:201:HEC:HBC3	0.66	1.67	18	12
1:A:95:ARG:NH2	2:A:201:HEC:HAA2	0.64	2.07	11	1
1:A:76:PRO:O	2:A:201:HEC:HAD1	0.64	1.92	4	3
1:A:91:ASP:O	1:A:95:ARG:HG2	0.62	1.95	14	1
1:A:55:CYS:SG	2:A:201:HEC:HMB1	0.61	2.36	18	15
1:A:106:PHE:CE2	2:A:201:HEC:HBB2	0.60	2.30	10	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ARG:HG2	1:A:115:ILE:HD13	0.60	1.73	9	4
1:A:58:CYS:HB3	2:A:201:HEC:C2C	0.59	2.28	9	6
1:A:114:ASP:O	1:A:118:LEU:HD23	0.58	1.98	11	3
1:A:51:TYR:HA	1:A:55:CYS:SG	0.57	2.39	14	13
1:A:119:VAL:O	1:A:123:ARG:HG2	0.56	2.00	9	1
1:A:95:ARG:NH1	2:A:201:HEC:HAA2	0.56	2.16	3	3
1:A:91:ASP:O	1:A:95:ARG:HG3	0.54	2.02	10	12
1:A:76:PRO:O	2:A:201:HEC:HBD1	0.54	2.02	7	1
1:A:81:VAL:HA	1:A:126:ALA:HB1	0.54	1.80	3	2
2:A:201:HEC:HBC3	2:A:201:HEC:CMC	0.53	2.34	16	6
1:A:100:ARG:HA	1:A:100:ARG:NE	0.53	2.18	6	3
1:A:59:HIS:ND1	1:A:80:LEU:HD21	0.52	2.19	17	1
1:A:43:SER:HA	1:A:117:ASP:CG	0.52	2.29	10	8
1:A:46:GLN:NE2	1:A:114:ASP:HA	0.52	2.20	10	1
1:A:51:TYR:OH	1:A:63:LEU:HD23	0.51	2.06	4	1
1:A:60:GLY:HA3	1:A:66:ASP:H	0.51	1.66	10	3
1:A:80:LEU:HD23	1:A:122:MET:SD	0.51	2.46	5	1
1:A:58:CYS:SG	2:A:201:HEC:HMC1	0.50	2.47	1	2
1:A:106:PHE:CZ	2:A:201:HEC:HBB2	0.50	2.41	13	1
1:A:103:MET:HB2	2:A:201:HEC:CHD	0.50	2.36	7	1
1:A:96:VAL:HA	1:A:103:MET:CE	0.50	2.37	19	1
1:A:36:PRO:HD2	1:A:116:TRP:CE2	0.49	2.42	18	1
2:A:201:HEC:CBC	2:A:201:HEC:CMC	0.49	2.89	3	4
1:A:43:SER:HA	1:A:117:ASP:OD2	0.49	2.07	3	4
1:A:46:GLN:O	1:A:49:VAL:HG12	0.49	2.08	5	2
1:A:115:ILE:O	1:A:119:VAL:HG12	0.49	2.08	11	3
1:A:29:ALA:O	1:A:33:ARG:HD3	0.48	2.08	19	3
2:A:201:HEC:CMC	2:A:201:HEC:CBC	0.48	2.90	16	2
1:A:55:CYS:SG	2:A:201:HEC:CMB	0.48	3.02	19	4
1:A:112:GLU:HB3	1:A:116:TRP:NE1	0.47	2.25	9	1
1:A:49:VAL:O	1:A:53:GLU:HG3	0.47	2.09	7	4
1:A:93:ALA:O	1:A:97:ARG:HG3	0.47	2.09	9	2
1:A:58:CYS:O	1:A:70:ALA:HB2	0.47	2.09	4	2
1:A:58:CYS:HB3	2:A:201:HEC:CMC	0.47	2.40	9	1
1:A:55:CYS:O	1:A:59:HIS:HB2	0.46	2.10	9	2
1:A:95:ARG:HG3	2:A:201:HEC:HMA1	0.46	1.85	6	1
1:A:95:ARG:O	1:A:99:GLY:HA2	0.46	2.10	9	1
1:A:93:ALA:HB1	1:A:116:TRP:CZ3	0.46	2.46	1	1
1:A:35:ASN:OD1	1:A:89:ASP:HB3	0.46	2.10	6	1
1:A:31:ILE:HG23	1:A:91:ASP:HB2	0.46	1.88	8	1
1:A:95:ARG:HD2	2:A:201:HEC:C2A	0.46	2.40	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ASP:HB2	1:A:75:PRO:HD3	0.46	1.88	3	3
1:A:37:ILE:HG21	1:A:117:ASP:OD2	0.45	2.10	18	2
1:A:113:ARG:HA	1:A:116:TRP:CE3	0.45	2.45	15	4
1:A:95:ARG:HD3	2:A:201:HEC:CAA	0.45	2.42	20	2
1:A:73:LEU:HD13	1:A:75:PRO:O	0.45	2.12	13	2
2:A:201:HEC:HMC1	2:A:201:HEC:CBC	0.45	2.38	3	2
1:A:97:ARG:HG2	1:A:115:ILE:CD1	0.45	2.41	2	3
1:A:50:LEU:CB	1:A:118:LEU:HD21	0.45	2.41	10	2
1:A:42:ARG:HG3	1:A:43:SER:N	0.45	2.26	19	5
2:A:201:HEC:HMD1	2:A:201:HEC:HBD2	0.45	1.89	9	1
1:A:118:LEU:HD13	2:A:201:HEC:CMB	0.45	2.42	20	1
1:A:84:ALA:N	1:A:85:PRO:HD2	0.45	2.26	9	5
1:A:59:HIS:ND1	1:A:80:LEU:HD11	0.44	2.27	2	1
1:A:103:MET:HB3	2:A:201:HEC:C4C	0.44	2.42	10	1
1:A:95:ARG:CZ	2:A:201:HEC:HAA2	0.44	2.42	11	2
1:A:95:ARG:HD2	2:A:201:HEC:CAA	0.44	2.43	15	1
1:A:78:ALA:HB1	1:A:83:HIS:CE1	0.44	2.48	5	1
1:A:30:GLU:O	1:A:33:ARG:HB2	0.44	2.12	16	1
1:A:74:ASP:HB3	1:A:75:PRO:HD3	0.44	1.89	9	2
1:A:110:LEU:HB3	1:A:114:ASP:HB2	0.43	1.90	12	1
1:A:92:LEU:O	1:A:96:VAL:HG23	0.43	2.12	11	2
1:A:100:ARG:O	1:A:102:PRO:HD2	0.43	2.13	14	1
1:A:43:SER:OG	1:A:117:ASP:HA	0.43	2.13	4	1
1:A:64:ARG:HD2	1:A:79:ASP:OD2	0.43	2.13	15	1
1:A:40:ASP:CG	1:A:41:ALA:H	0.43	2.22	10	3
1:A:63:LEU:HB3	1:A:80:LEU:HB2	0.43	1.90	13	1
1:A:107:GLY:HA2	1:A:115:ILE:HD11	0.42	1.90	9	1
1:A:55:CYS:HA	2:A:201:HEC:CHC	0.42	2.45	6	2
1:A:122:MET:HE1	2:A:201:HEC:CMA	0.42	2.45	11	1
1:A:92:LEU:O	2:A:201:HEC:HMA2	0.42	2.15	15	1
1:A:80:LEU:HD12	1:A:80:LEU:H	0.41	1.74	5	1
1:A:47:GLY:O	1:A:51:TYR:HB2	0.41	2.15	7	2
1:A:43:SER:HB3	1:A:120:ASN:HB2	0.41	1.92	14	1
1:A:103:MET:HB2	2:A:201:HEC:C4C	0.41	2.46	7	1
1:A:80:LEU:HD13	1:A:122:MET:SD	0.41	2.55	7	2
1:A:111:ASP:HB2	1:A:114:ASP:OD1	0.41	2.16	11	1
1:A:59:HIS:HD1	1:A:80:LEU:HD11	0.41	1.75	13	1
1:A:69:ASP:O	1:A:73:LEU:HG	0.41	2.15	7	1
1:A:27:PRO:O	1:A:31:ILE:HG13	0.41	2.15	15	1
1:A:100:ARG:H	1:A:103:MET:HG3	0.41	1.76	18	1
1:A:80:LEU:HD12	1:A:80:LEU:N	0.40	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:MET:CE	2:A:201:HEC:HMA2	0.40	2.42	13	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/125 (84%)	99±1 (95±1%)	5±1 (5±1%)	0±1 (0±1%)	44	80
All	All	2100/2500 (84%)	1986 (95%)	109 (5%)	5 (0%)	44	80

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	74	ASP	2
1	A	100	ARG	2
1	A	65	GLY	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/98 (85%)	82±1 (98±1%)	1±1 (2±1%)	54	92
All	All	1660/1960 (85%)	1633 (98%)	27 (2%)	54	92

All 12 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	46	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	116	TRP	5
1	A	59	HIS	2
1	A	35	ASN	2
1	A	96	VAL	2
1	A	62	THR	2
1	A	66	ASP	2
1	A	91	ASP	1
1	A	83	HIS	1
1	A	74	ASP	1
1	A	100	ARG	1
1	A	119	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEC	A	201	1	50,50,50	0.69±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics

could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	201	1	68,82,82	0.87±0.01	1±1 (1±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	201	1	1±0,1,7,7	0±0,14,54,54	-

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	201	HEC	CAD-CBD-CGD	2.40	108.45	113.60	9	12
2	A	201	HEC	CAA-CBA-CGA	2.35	108.56	113.60	6	7

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	201	HEC	NA	20

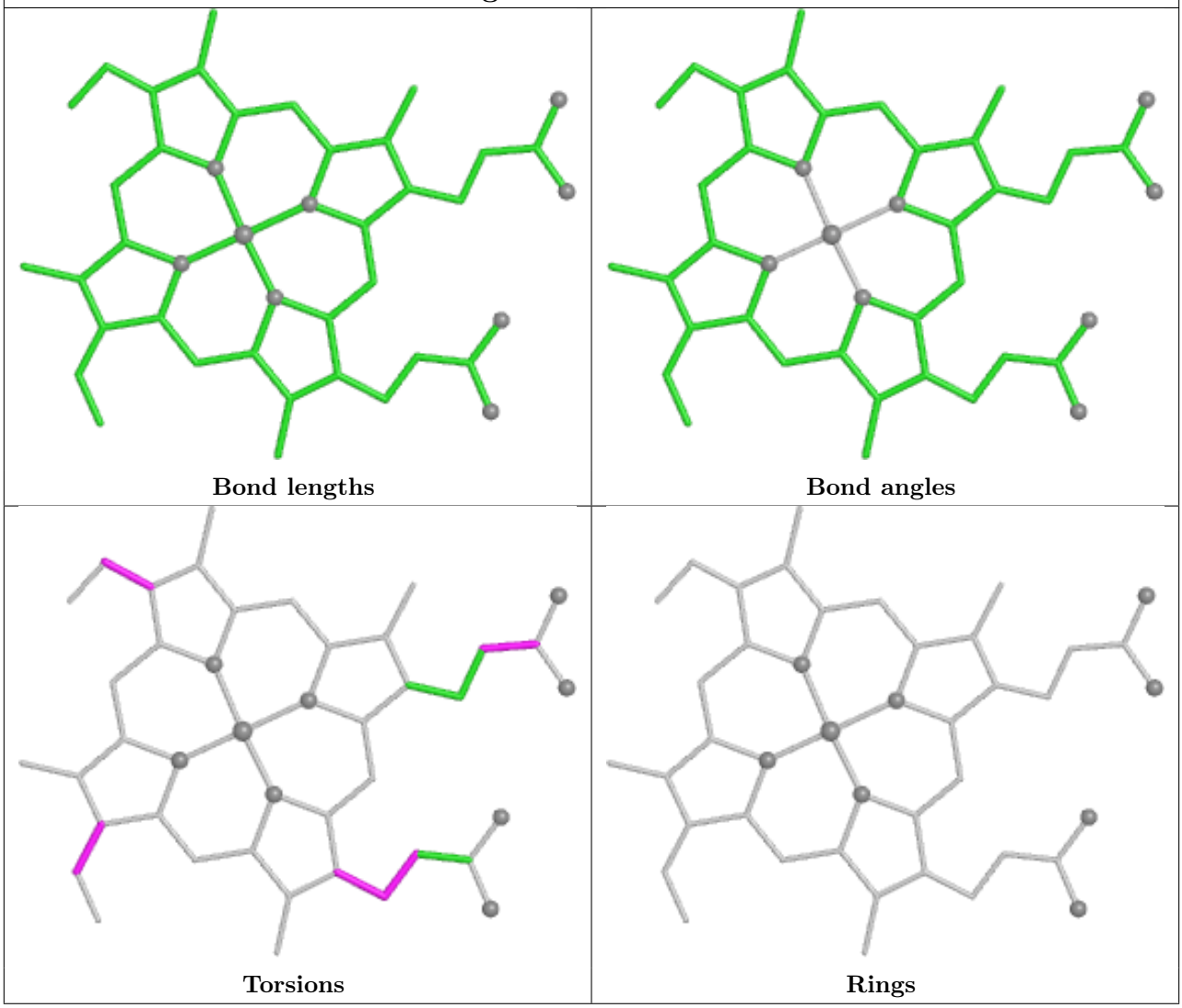
There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEC A 201



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1184
Number of shifts mapped to atoms	1184
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	30

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	110	-0.81 ± 0.19	Should be checked
$^{13}C_{\beta}$	98	0.40 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	102	-0.81 ± 0.40	Should be applied
^{15}N	102	1.16 ± 0.48	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1090 atoms were assigned a chemical shift out of a possible 1374. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	493/516 (96%)	205/211 (97%)	195/210 (93%)	93/95 (98%)
Sidechain	595/753 (79%)	407/486 (84%)	184/233 (79%)	4/34 (12%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/105 (2%)	1/52 (2%)	0/39 (0%)	1/14 (7%)
Overall	1090/1374 (79%)	613/749 (82%)	379/482 (79%)	98/143 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1173 atoms were assigned a chemical shift out of a possible 1488. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	537/575 (93%)	223/237 (94%)	212/232 (91%)	102/106 (96%)
Sidechain	632/796 (79%)	432/514 (84%)	195/247 (79%)	5/35 (14%)
Aromatic	4/117 (3%)	2/58 (3%)	0/44 (0%)	2/15 (13%)
Overall	1173/1488 (79%)	657/809 (81%)	407/523 (78%)	109/156 (70%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	80	LEU	HG	6.00	-0.13 – 3.16	13.7
1	A	96	VAL	HG21	-2.28	-0.58 – 2.19	-11.1
1	A	96	VAL	HG22	-2.28	-0.58 – 2.19	-11.1
1	A	96	VAL	HG23	-2.28	-0.58 – 2.19	-11.1
1	A	99	GLY	HA3	7.41	2.08 – 5.71	9.7
1	A	80	LEU	HD21	3.40	-0.65 – 2.13	9.6
1	A	80	LEU	HD22	3.40	-0.65 – 2.13	9.6
1	A	80	LEU	HD23	3.40	-0.65 – 2.13	9.6
1	A	77	VAL	HG11	-1.55	-0.48 – 2.12	-9.1
1	A	77	VAL	HG12	-1.55	-0.48 – 2.12	-9.1
1	A	77	VAL	HG13	-1.55	-0.48 – 2.12	-9.1
1	A	99	GLY	HA2	6.84	2.15 – 5.77	8.0
1	A	96	VAL	HG11	-1.23	-0.48 – 2.12	-7.9
1	A	96	VAL	HG12	-1.23	-0.48 – 2.12	-7.9
1	A	96	VAL	HG13	-1.23	-0.48 – 2.12	-7.9
1	A	104	PRO	HG2	4.00	0.41 – 3.45	6.8
1	A	35	ASN	HA	2.38	2.91 – 6.40	-6.5
1	A	36	PRO	HD2	1.47	1.93 – 5.38	-6.3
1	A	118	LEU	HG	-0.55	-0.13 – 3.16	-6.3
1	A	104	PRO	HG3	3.85	0.33 – 3.48	6.2
1	A	80	LEU	HD11	2.42	-0.61 – 2.12	6.1
1	A	80	LEU	HD12	2.42	-0.61 – 2.12	6.1

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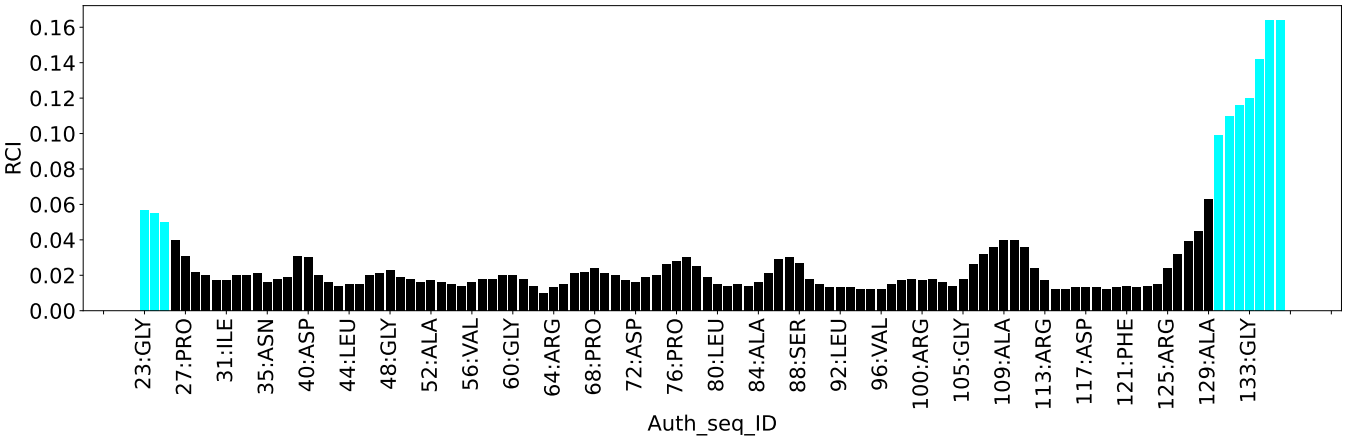
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	80	LEU	HD13	2.42	-0.61 – 2.12	6.1
1	A	55	CYS	HB2	0.34	0.81 – 5.11	-6.1
1	A	80	LEU	HB3	3.57	-0.26 – 3.31	5.7
1	A	118	LEU	HB2	-0.27	-0.07 – 3.30	-5.6
1	A	105	GLY	HA2	5.97	2.15 – 5.77	5.5
1	A	102	PRO	HG3	0.21	0.33 – 3.48	-5.4
1	A	100	ARG	HD3	1.78	1.81 – 4.39	-5.1
1	A	104	PRO	HA	6.01	2.78 – 6.00	5.0

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1166
Intra-residue (|i-j|=0)	530
Sequential (|i-j|=1)	282
Medium range (|i-j|>1 and |i-j|<5)	206
Long range (|i-j|≥5)	134
Inter-chain	14
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	167
Number of unmapped restraints	0
Number of restraints per residue	10.6
Number of long range restraints per residue[1]	1.1

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	8.8	0.2
0.2-0.5 (Medium)	14.2	0.5
>0.5 (Large)	41.5	3.48

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	25.5	9.93
10.0-20.0 (Medium)	1.6	16.79
>20.0 (Large)	2.0	62.5

9 Distance violation analysis (i)

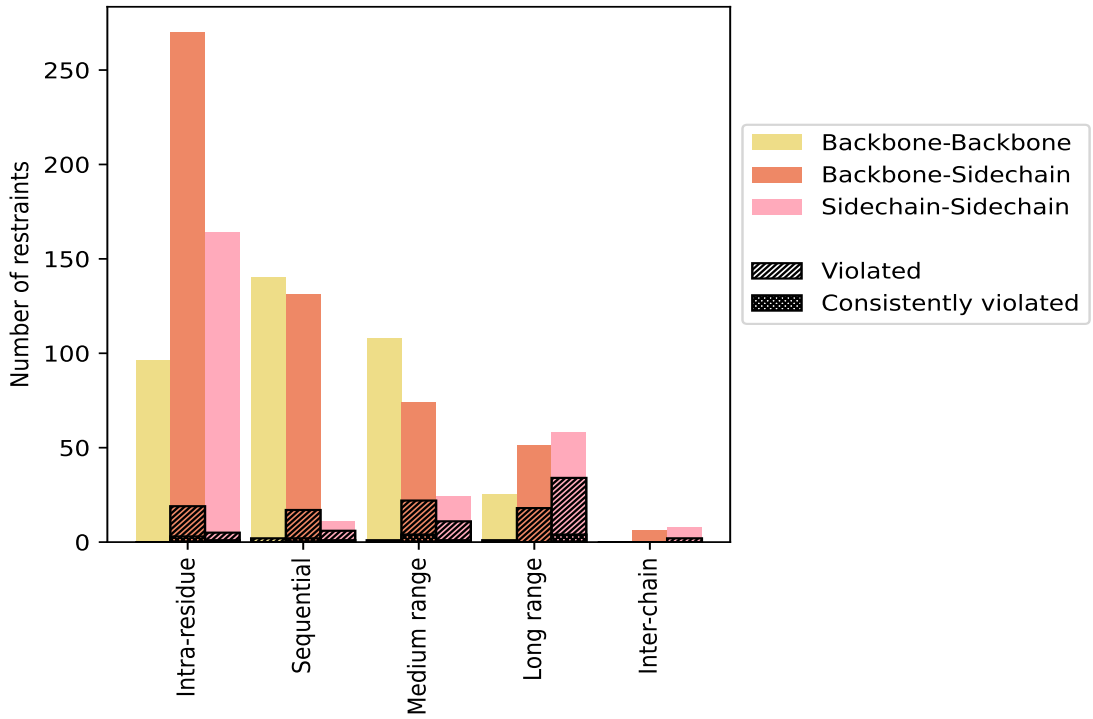
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	530	45.5	24	4.5	2.1	4	0.8	0.3
Backbone-Backbone	96	8.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	270	23.2	19	7.0	1.6	3	1.1	0.3
Sidechain-Sidechain	164	14.1	5	3.0	0.4	1	0.6	0.1
Sequential (|i-j|=1)	282	24.2	25	8.9	2.1	3	1.1	0.3
Backbone-Backbone	140	12.0	2	1.4	0.2	0	0.0	0.0
Backbone-Sidechain	131	11.2	17	13.0	1.5	2	1.5	0.2
Sidechain-Sidechain	11	0.9	6	54.5	0.5	1	9.1	0.1
Medium range (|i-j|>1 & |i-j|<5)	206	17.7	34	16.5	2.9	5	2.4	0.4
Backbone-Backbone	108	9.3	1	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	74	6.3	22	29.7	1.9	4	5.4	0.3
Sidechain-Sidechain	24	2.1	11	45.8	0.9	1	4.2	0.1
Long range (|i-j|≥5)	134	11.5	53	39.6	4.5	4	3.0	0.3
Backbone-Backbone	25	2.1	1	4.0	0.1	0	0.0	0.0
Backbone-Sidechain	51	4.4	18	35.3	1.5	0	0.0	0.0
Sidechain-Sidechain	58	5.0	34	58.6	2.9	4	6.9	0.3
Inter-chain	14	1.2	2	14.3	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	0.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	0.7	2	25.0	0.2	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1166	100.0	138	11.8	11.8	16	1.4	1.4
Backbone-Backbone	369	31.6	4	1.1	0.3	0	0.0	0.0
Backbone-Sidechain	532	45.6	76	14.3	6.5	9	1.7	0.8
Sidechain-Sidechain	265	22.7	58	21.9	5.0	7	2.6	0.6

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å
are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	14	12	20	24	0	70	0.87	3.14	0.63	0.78
2	9	8	16	14	0	47	0.74	2.47	0.59	0.55
3	14	11	17	23	0	65	0.75	1.78	0.54	0.57
4	16	13	19	22	0	70	0.85	2.97	0.62	0.74
5	10	9	18	19	1	57	0.88	2.87	0.64	0.79
6	12	11	24	17	0	64	0.85	2.87	0.62	0.7
7	16	11	19	27	0	73	1.0	3.26	0.63	0.96
8	16	10	24	25	1	76	1.01	3.17	0.67	0.93
9	12	8	15	16	0	51	0.84	2.96	0.67	0.72
10	12	10	22	23	1	68	1.04	3.22	0.73	1.01

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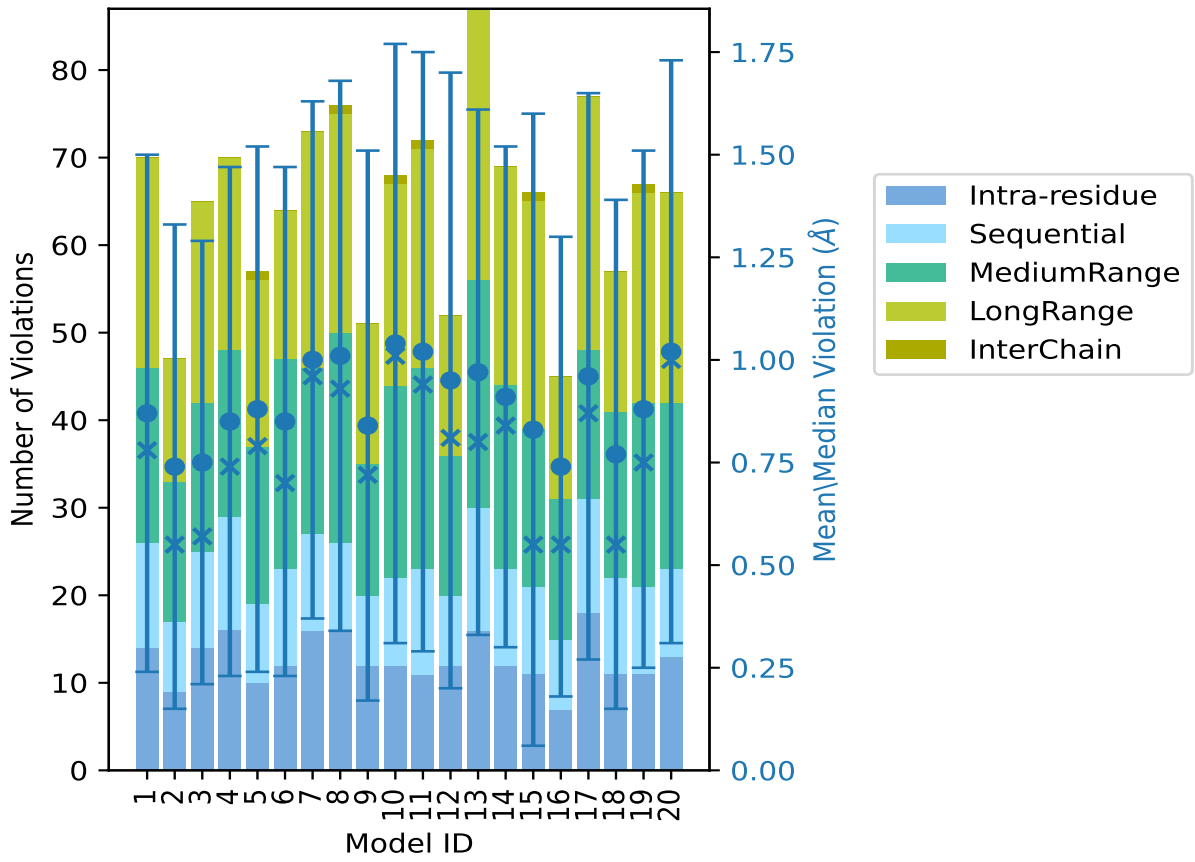
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	11	12	23	25	1	72	1.02	3.37	0.73	0.94
12	12	8	16	16	0	52	0.95	3.07	0.75	0.81
13	16	14	26	31	0	87	0.97	3.2	0.64	0.8
14	12	11	21	25	0	69	0.91	2.54	0.61	0.84
15	11	10	18	26	1	66	0.83	3.48	0.77	0.55
16	7	8	16	14	0	45	0.74	2.14	0.56	0.55
17	18	13	17	29	0	77	0.96	3.19	0.69	0.87
18	11	11	19	16	0	57	0.77	2.64	0.62	0.55
19	11	10	21	24	1	67	0.88	2.4	0.63	0.75
20	13	10	19	24	0	66	1.02	3.05	0.71	1.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

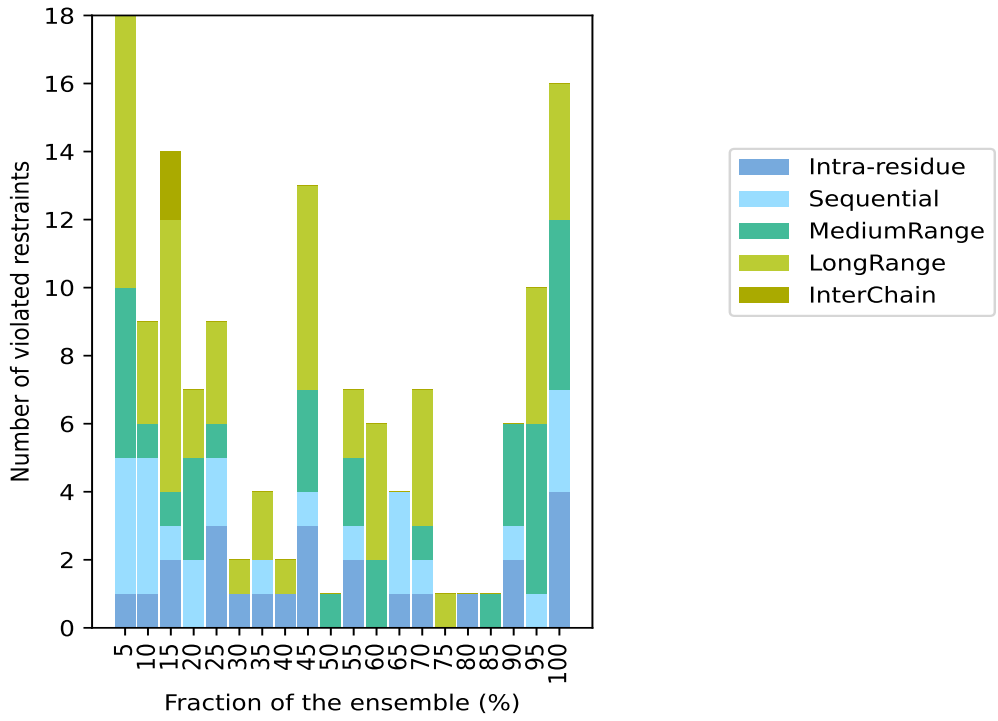
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1028(IR:506, SQ:257, MR:172, LR:81, IC:12) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	4	5	8	0	18	1	5.0
1	4	1	3	0	9	2	10.0
2	1	1	8	2	14	3	15.0
0	2	3	2	0	7	4	20.0
3	2	1	3	0	9	5	25.0
1	0	0	1	0	2	6	30.0
1	1	0	2	0	4	7	35.0
1	0	0	1	0	2	8	40.0
3	1	3	6	0	13	9	45.0
0	0	1	0	0	1	10	50.0
2	1	2	2	0	7	11	55.0
0	0	2	4	0	6	12	60.0
1	3	0	0	0	4	13	65.0
1	1	1	4	0	7	14	70.0
0	0	0	1	0	1	15	75.0
1	0	0	0	0	1	16	80.0
0	0	1	0	0	1	17	85.0
2	1	3	0	0	6	18	90.0
0	1	5	4	0	10	19	95.0
4	3	5	4	0	16	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

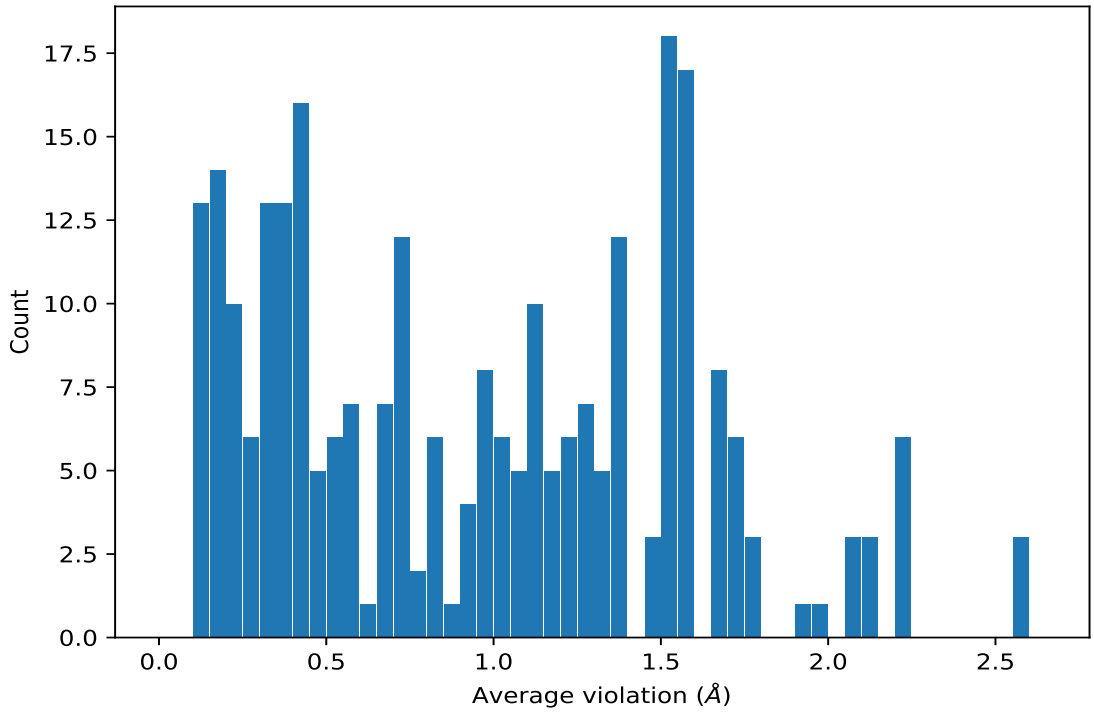
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of theviolation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	20	2.56	0.55	2.59
(1,702)	1:50:A:LEU:HD13	1:46:A:GLN:HG3	20	2.56	0.55	2.59
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	20	2.56	0.55	2.59
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	20	1.95	0.13	1.96
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	20	1.57	1.48	0.4
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	20	1.57	1.48	0.4
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	20	1.57	1.48	0.4
(1,963)	1:118:A:LEU:HD23	1:51:A:TYR:HB3	20	1.49	0.79	1.2
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	20	1.49	0.79	1.2
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	20	1.49	0.79	1.2
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	20	1.36	0.09	1.38
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	20	1.36	0.09	1.38
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	20	1.36	0.09	1.38
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	20	1.14	0.04	1.14
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	20	1.12	0.3	1.08
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	20	1.12	0.3	1.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1091)	1:96:A:VAL:HG13	1:115:A:ILE:HG13	20	1.12	0.3	1.08
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	20	0.98	0.04	0.98
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	20	0.96	0.57	0.62
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	20	0.96	0.57	0.62
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	20	0.96	0.57	0.62
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	20	0.92	0.14	0.93
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	20	0.84	0.1	0.82
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	20	0.72	0.12	0.76
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	20	0.55	0.01	0.55
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	20	0.55	0.01	0.55
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	20	0.55	0.01	0.55
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	20	0.31	0.02	0.32
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	20	0.3	0.06	0.3
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	20	0.16	0.03	0.16
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD21	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD23	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD23	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD22	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD23	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD22	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD21	19	1.58	0.19	1.61
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD21	19	1.58	0.19	1.61
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD11	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD12	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD11	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD13	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD13	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD12	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD12	19	1.52	0.23	1.59
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD11	19	1.52	0.23	1.59
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	19	1.32	0.49	1.26
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD13	19	1.32	0.49	1.26
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	19	1.32	0.49	1.26
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	19	1.29	0.69	1.62
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	19	1.28	0.57	1.34
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD13	19	1.28	0.57	1.34
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	19	1.28	0.57	1.34
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	19	1.1	0.18	1.11
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD22	19	1.1	0.18	1.11
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	19	1.1	0.18	1.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	19	0.61	0.16	0.63
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	19	0.45	0.08	0.45
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	19	0.45	0.08	0.45
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	19	0.45	0.08	0.45
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	19	0.42	0.17	0.41
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	19	0.39	0.18	0.31
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD23	19	0.39	0.18	0.31
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	19	0.39	0.18	0.31
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	18	1.71	0.05	1.72
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	18	1.71	0.05	1.72
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	18	1.71	0.05	1.72
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	18	1.53	0.14	1.55
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	18	1.53	0.14	1.55
(1,766)	1:49:A:VAL:HG11	1:46:A:GLN:HA	18	1.53	0.14	1.55
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	18	1.37	0.02	1.38
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	18	1.37	0.02	1.38
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG13	18	1.37	0.02	1.38
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	18	0.47	0.26	0.4
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	18	0.23	0.09	0.21
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	18	0.23	0.09	0.21
(1,836)	1:110:A:LEU:HD21	1:106:A:PHE:HB3	18	0.23	0.09	0.21
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	18	0.17	0.02	0.18
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	17	0.77	0.43	0.65
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	16	0.21	0.09	0.18
(1,704)	1:50:A:LEU:HD11	1:50:A:LEU:H	16	0.21	0.09	0.18
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	16	0.21	0.09	0.18
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	15	0.34	0.14	0.3
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	14	1.56	0.16	1.54
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	14	1.56	0.16	1.54
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG12	14	1.56	0.16	1.54
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	14	1.52	0.28	1.4
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	14	1.52	0.28	1.4
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG12	14	1.52	0.28	1.4
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	14	1.25	0.19	1.24
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	14	1.25	0.19	1.24
(1,1074)	1:81:A:VAL:HG11	1:64:A:ARG:HG2	14	1.25	0.19	1.24
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG11	14	1.2	0.02	1.19
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG13	14	1.2	0.02	1.19
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	14	1.2	0.02	1.19
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	14	1.1	0.09	1.1
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG11	14	1.1	0.09	1.1
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG13	14	1.1	0.09	1.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	14	1.04	0.13	1.04
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	14	1.04	0.13	1.04
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG11	14	1.04	0.13	1.04
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	14	0.59	0.31	0.5
(1,893)	1:26:A:VAL:HG11	1:27:A:PRO:HD3	13	1.38	0.51	1.55
(1,893)	1:26:A:VAL:HG13	1:27:A:PRO:HD3	13	1.38	0.51	1.55
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	13	1.38	0.51	1.55
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	13	0.37	0.12	0.35
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	13	0.25	0.09	0.27
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	13	0.25	0.09	0.27
(1,1031)	1:41:A:ALA:HB1	1:40:A:ASP:HB3	13	0.25	0.09	0.27
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	13	0.14	0.02	0.13
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	12	0.81	0.48	1.04
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG12	12	0.81	0.48	1.04
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG11	12	0.81	0.48	1.04
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	12	0.45	0.3	0.38
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	12	0.4	0.21	0.34
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB3	12	0.4	0.21	0.34
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB2	12	0.4	0.21	0.34
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB1	12	0.4	0.21	0.34
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB2	12	0.4	0.21	0.34
(1,709)	1:81:A:VAL:HG22	1:129:A:ALA:HB3	12	0.4	0.21	0.34
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	12	0.38	0.17	0.34
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	12	0.35	0.15	0.31
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	12	0.23	0.08	0.24
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG22	12	0.23	0.08	0.24
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG23	12	0.23	0.08	0.24
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG21	11	1.75	0.27	1.76
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	11	1.75	0.27	1.76
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG22	11	1.75	0.27	1.76
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG11	11	1.52	0.29	1.51
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	11	1.52	0.29	1.51
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG13	11	1.52	0.29	1.51
(1,892)	1:26:A:VAL:HG11	1:27:A:PRO:HD2	11	1.21	0.14	1.25
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	11	1.21	0.14	1.25
(1,892)	1:26:A:VAL:HG13	1:27:A:PRO:HD2	11	1.21	0.14	1.25
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG23	11	0.67	0.05	0.68
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	11	0.67	0.05	0.68
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG21	11	0.67	0.05	0.68
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	11	0.52	0.22	0.5
(1,879)	1:78:A:ALA:HB2	1:83:A:HIS:HB3	11	0.52	0.22	0.5
(1,879)	1:78:A:ALA:HB3	1:83:A:HIS:HB3	11	0.52	0.22	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG12	11	0.32	0.01	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	11	0.32	0.01	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG11	11	0.32	0.01	0.33
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG12	11	0.25	0.08	0.25
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	11	0.25	0.08	0.25
(1,843)	1:73:A:LEU:HD12	1:70:A:ALA:HB3	10	0.36	0.2	0.29
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB3	10	0.36	0.2	0.29
(1,843)	1:73:A:LEU:HD13	1:70:A:ALA:HB3	10	0.36	0.2	0.29
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB1	10	0.36	0.2	0.29
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG23	9	2.22	0.12	2.21
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG21	9	2.22	0.12	2.21
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG22	9	2.22	0.12	2.21
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD12	9	2.11	0.06	2.11
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD13	9	2.11	0.06	2.11
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD11	9	2.11	0.06	2.11
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG22	9	2.09	0.14	2.06
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG23	9	2.09	0.14	2.06
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG21	9	2.09	0.14	2.06
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	9	1.69	0.1	1.71
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG22	9	1.69	0.1	1.71
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG23	9	1.69	0.1	1.71
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD12	9	1.69	0.02	1.68
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD11	9	1.69	0.02	1.68
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD13	9	1.69	0.02	1.68
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD12	9	1.38	0.1	1.35
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD11	9	1.38	0.1	1.35
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD13	9	1.38	0.1	1.35
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD11	9	1.17	0.08	1.16
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD13	9	1.17	0.08	1.16
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD12	9	1.17	0.08	1.16
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD23	9	1.07	0.14	1.12
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD21	9	1.07	0.14	1.12
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD22	9	1.07	0.14	1.12
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	9	0.93	0.05	0.94
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG22	9	0.93	0.05	0.94
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG23	9	0.93	0.05	0.94
(1,870)	1:44:A:LEU:HD11	1:124:A:ASP:HB2	9	0.65	0.13	0.6
(1,870)	1:44:A:LEU:HD13	1:124:A:ASP:HB2	9	0.65	0.13	0.6
(1,870)	1:44:A:LEU:HD12	1:124:A:ASP:HB2	9	0.65	0.13	0.6
(1,791)	1:44:A:LEU:HD21	1:44:A:LEU:HB2	9	0.54	0.01	0.55
(1,791)	1:44:A:LEU:HD22	1:44:A:LEU:HB2	9	0.54	0.01	0.55
(1,791)	1:44:A:LEU:HD23	1:44:A:LEU:HB2	9	0.54	0.01	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG11	9	0.44	0.24	0.38
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	9	0.44	0.24	0.38
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG12	9	0.44	0.24	0.38
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	9	0.18	0.05	0.21
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	8	2.21	0.28	2.28
(1,964)	1:56:A:VAL:HG22	1:61:A:GLU:HA	8	2.21	0.28	2.28
(1,964)	1:56:A:VAL:HG23	1:61:A:GLU:HA	8	2.21	0.28	2.28
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	8	0.98	0.02	0.98
(1,965)	1:56:A:VAL:HG21	1:56:A:VAL:HA	8	0.98	0.02	0.98
(1,965)	1:56:A:VAL:HG22	1:56:A:VAL:HA	8	0.98	0.02	0.98
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG13	7	0.55	0.19	0.5
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG12	7	0.55	0.19	0.5
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG11	7	0.55	0.19	0.5
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG21	7	0.31	0.24	0.19
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG22	7	0.31	0.24	0.19
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG23	7	0.31	0.24	0.19
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	7	0.19	0.05	0.22
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD12	7	0.17	0.05	0.17
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD11	7	0.17	0.05	0.17
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD13	7	0.17	0.05	0.17
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	6	0.44	0.26	0.35
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	6	0.18	0.01	0.18
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD13	5	1.67	0.02	1.67
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD11	5	1.67	0.02	1.67
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD13	5	1.55	0.03	1.56
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD11	5	1.55	0.03	1.56
(1,1056)	1:63:A:LEU:HD21	1:125:A:ARG:HB3	5	1.18	0.49	1.1
(1,1056)	1:63:A:LEU:HD23	1:125:A:ARG:HB3	5	1.18	0.49	1.1
(1,1055)	1:63:A:LEU:HD21	1:125:A:ARG:HB2	5	0.82	0.28	0.68
(1,1055)	1:63:A:LEU:HD23	1:125:A:ARG:HB2	5	0.82	0.28	0.68
(1,1133)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	5	0.73	0.01	0.73
(1,1133)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	5	0.73	0.01	0.73
(1,1133)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	5	0.73	0.01	0.73
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD12	5	0.71	0.03	0.72
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD13	5	0.71	0.03	0.72
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD11	5	0.71	0.03	0.72
(1,880)	1:115:A:ILE:HD12	1:107:A:GLY:HA3	5	0.35	0.12	0.4
(1,880)	1:115:A:ILE:HD13	1:107:A:GLY:HA3	5	0.35	0.12	0.4
(1,880)	1:115:A:ILE:HD11	1:107:A:GLY:HA3	5	0.35	0.12	0.4
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG11	5	0.19	0.11	0.14
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG13	5	0.19	0.11	0.14
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	5	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,539)	1:89:A:ASP:H	1:35:A:ASN:HD22	4	1.3	0.48	1.34
(1,430)	1:42:A:ARG:H	1:43:A:SER:HB3	4	0.85	0.1	0.84
(1,602)	1:116:A:TRP:H	1:112:A:GLU:HB2	4	0.44	0.33	0.42
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD21	4	0.44	0.27	0.36
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD22	4	0.44	0.27	0.36
(1,402)	1:24:A:TRP:HE1	1:23:A:GLY:HA3	4	0.28	0.1	0.32
(1,785)	1:51:A:TYR:HA	1:55:A:CYS:HB3	4	0.18	0.08	0.16
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB3	4	0.12	0.02	0.12
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB1	4	0.12	0.02	0.12
(1,7)	2:201:A:HEC:HBB3	1:96:A:VAL:HG11	3	1.93	0.25	2.05
(1,4)	1:118:A:LEU:HD23	2:201:A:HEC:HMB1	3	1.71	0.16	1.71
(1,4)	1:118:A:LEU:HD22	2:201:A:HEC:HMB2	3	1.71	0.16	1.71
(1,4)	1:118:A:LEU:HD21	2:201:A:HEC:HMB1	3	1.71	0.16	1.71
(1,1097)	1:102:A:PRO:HB2	1:73:A:LEU:HD12	3	1.3	0.15	1.2
(1,972)	1:93:A:ALA:HA	1:96:A:VAL:HG21	3	1.05	0.1	1.08
(1,972)	1:93:A:ALA:HA	1:96:A:VAL:HG22	3	1.05	0.1	1.08
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD23	3	1.04	0.1	1.06
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD22	3	1.04	0.1	1.06
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD21	3	1.04	0.1	1.06
(1,1088)	1:106:A:PHE:HB2	1:96:A:VAL:HG12	3	0.96	0.12	0.92
(1,1066)	1:73:A:LEU:HD12	1:102:A:PRO:HB3	3	0.75	0.07	0.8
(1,1040)	1:118:A:LEU:HD22	1:51:A:TYR:HB2	3	0.73	0.06	0.7
(1,1040)	1:118:A:LEU:HD21	1:51:A:TYR:HB2	3	0.73	0.06	0.7
(1,1040)	1:118:A:LEU:HD23	1:51:A:TYR:HB2	3	0.73	0.06	0.7
(1,865)	1:96:A:VAL:H	1:96:A:VAL:HG23	3	0.7	0.03	0.7
(1,865)	1:96:A:VAL:H	1:96:A:VAL:HG21	3	0.7	0.03	0.7
(1,800)	1:96:A:VAL:HG13	1:103:A:MET:HE2	3	0.67	0.23	0.79
(1,844)	1:73:A:LEU:HB3	1:73:A:LEU:HD12	3	0.15	0.01	0.15
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD11	3	0.14	0.03	0.15
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD12	3	0.14	0.03	0.15
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD13	3	0.14	0.03	0.15
(1,952)	1:109:A:ALA:HB1	1:110:A:LEU:HD23	3	0.14	0.03	0.13
(1,952)	1:109:A:ALA:HB1	1:110:A:LEU:HD21	3	0.14	0.03	0.13
(1,952)	1:109:A:ALA:HB2	1:110:A:LEU:HD21	3	0.14	0.03	0.13
(1,1054)	1:63:A:LEU:HB3	1:80:A:LEU:HB2	3	0.11	0.01	0.11
(1,1052)	1:61:A:GLU:HG3	1:56:A:VAL:HG21	2	0.42	0.03	0.42
(1,1052)	1:61:A:GLU:HG3	1:56:A:VAL:HG22	2	0.42	0.03	0.42
(1,403)	1:25:A:GLU:H	1:100:A:ARG:HD2	2	0.34	0.05	0.34
(1,502)	1:70:A:ALA:H	1:73:A:LEU:HD13	2	0.32	0.05	0.32
(1,502)	1:70:A:ALA:H	1:73:A:LEU:HD11	2	0.32	0.05	0.32
(1,580)	1:106:A:PHE:H	1:96:A:VAL:HG12	2	0.3	0.01	0.3
(1,782)	1:125:A:ARG:HD2	1:125:A:ARG:HA	2	0.24	0.02	0.24

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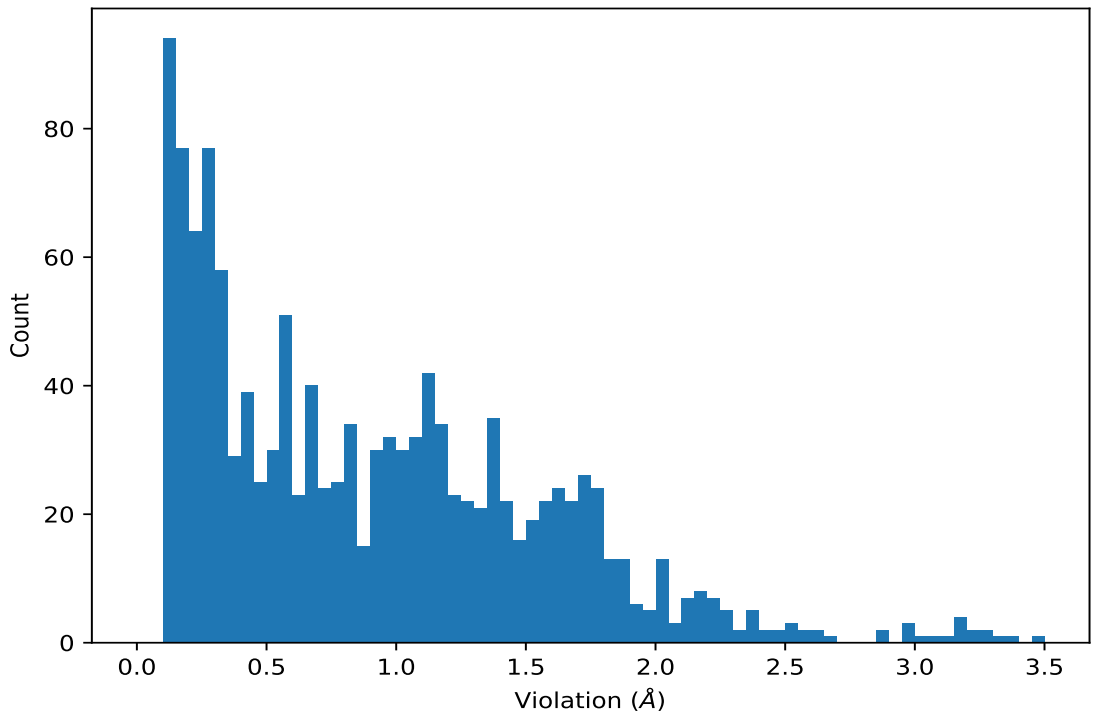
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,78)	1:37:A:ILE:H	1:36:A:PRO:HD3	2	0.18	0.02	0.18
(1,58)	1:60:A:GLY:H	1:59:A:HIS:H	2	0.15	0.01	0.15
(1,53)	1:41:A:ALA:H	1:40:A:ASP:HB3	2	0.14	0.02	0.14
(1,309)	1:74:A:ASP:H	1:73:A:LEU:HB2	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	15	3.48
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	11	3.37
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	11	3.32
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	15	3.3
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	7	3.26
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	10	3.22
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	13	3.2
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	17	3.19
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	10	3.17
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	8	3.17
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	17	3.16
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	1	3.14
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	12	3.07
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	20	3.05
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	4	2.97
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	9	2.96
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	15	2.95
(1,702)	1:50:A:LEU:HD13	1:46:A:GLN:HG3	5	2.87
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	6	2.87
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	20	2.67
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	18	2.64
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	8	2.61
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	12	2.57
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	7	2.56
(1,964)	1:56:A:VAL:HG22	1:61:A:GLU:HA	18	2.54
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	14	2.54
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	1	2.53
(1,702)	1:50:A:LEU:HD13	1:46:A:GLN:HG3	2	2.47
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	10	2.46
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	13	2.44
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG22	8	2.43
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	19	2.4
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	9	2.4
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG22	17	2.38
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	20	2.36
(1,702)	1:50:A:LEU:HD13	1:46:A:GLN:HG3	13	2.35
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG23	6	2.33
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	12	2.31
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	15	2.3
(1,702)	1:50:A:LEU:HD13	1:46:A:GLN:HG3	11	2.3
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG21	19	2.3
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	4	2.28
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	14	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG22	5	2.24
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG22	14	2.23
(1,964)	1:56:A:VAL:HG22	1:61:A:GLU:HA	7	2.21
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG22	10	2.21
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG21	13	2.21
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG22	11	2.2
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD12	7	2.2
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	20	2.19
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG21	6	2.19
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	10	2.18
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	15	2.18
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD11	12	2.18
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	20	2.17
(1,7)	2:201:A:HEC:HBB3	1:96:A:VAL:HG11	5	2.16
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	12	2.15
(1,702)	1:50:A:LEU:HD12	1:46:A:GLN:HG3	16	2.14
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD13	20	2.13
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD13	8	2.12
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG21	8	2.11
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD13	11	2.11
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD12	15	2.11
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD12	17	2.1
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG23	14	2.09
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	16	2.06
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG23	19	2.06
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	8	2.05
(1,7)	2:201:A:HEC:HBB3	1:96:A:VAL:HG11	8	2.05
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	10	2.04
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	1	2.02
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	4	2.02
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG23	13	2.02
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	11	2.01
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	20	2.01
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG21	11	2.01
(1,605)	1:116:A:TRP:H	1:119:A:VAL:HG23	5	2.01
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	12	2.01
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD11	13	2.01
(1,114)	1:121:A:PHE:H	1:44:A:LEU:HD12	10	2.0
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	19	1.99
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	1	1.98
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	12	1.97
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG21	10	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	13	1.96
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	17	1.95
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	10	1.94
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG11	1	1.94
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	20	1.93
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	20	1.93
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG13	13	1.91
(1,539)	1:89:A:ASP:H	1:35:A:ASN:HD22	5	1.9
(1,4)	1:118:A:LEU:HD23	2:201:A:HEC:HMB1	10	1.9
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG21	4	1.89
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	9	1.88
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	13	1.88
(1,610)	1:117:A:ASP:H	1:119:A:VAL:HG21	17	1.88
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD13	2	1.88
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD13	11	1.88
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	19	1.87
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	18	1.87
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD11	11	1.87
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD21	8	1.86
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	10	1.85
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	2	1.84
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	5	1.83
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	13	1.83
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	6	1.83
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	18	1.83
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	5	1.82
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	8	1.81
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	8	1.81
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD21	17	1.81
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	7	1.81
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	12	1.81
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG22	6	1.8
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	2	1.8
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	4	1.79
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	14	1.79
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD13	9	1.79
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	6	1.79
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	16	1.79
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	3	1.78
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG22	14	1.78
(1,964)	1:56:A:VAL:HG21	1:61:A:GLU:HA	9	1.77
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	4	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD23	9	1.76
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG21	1	1.76
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	14	1.76
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	15	1.76
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	19	1.76
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	6	1.75
(1,1056)	1:63:A:LEU:HD21	1:125:A:ARG:HB3	3	1.75
(1,964)	1:56:A:VAL:HG23	1:61:A:GLU:HA	17	1.75
(1,893)	1:26:A:VAL:HG11	1:27:A:PRO:HD3	1	1.75
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	19	1.75
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD11	19	1.75
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	10	1.75
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	11	1.75
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	17	1.75
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	17	1.75
(1,1056)	1:63:A:LEU:HD21	1:125:A:ARG:HB3	7	1.74
(1,778)	1:47:A:GLY:HA3	1:50:A:LEU:HB3	5	1.74
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG23	19	1.74
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	7	1.74
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	14	1.74
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD12	12	1.73
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD21	1	1.73
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	20	1.73
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD13	13	1.73
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	9	1.73
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	10	1.72
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG12	11	1.72
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD23	4	1.72
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	3	1.72
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	1	1.72
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	9	1.72
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	20	1.72
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	11	1.72
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	7	1.72
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	4	1.72
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD11	11	1.71
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD11	20	1.71
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD22	7	1.71
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	3	1.71
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	8	1.71
(1,4)	1:118:A:LEU:HD22	2:201:A:HEC:HMB2	11	1.71
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	18	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD11	17	1.7
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	12	1.7
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	13	1.69
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD13	10	1.69
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	11	1.69
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	11	1.69
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD13	13	1.69
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	18	1.69
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD11	8	1.68
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD12	13	1.68
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD13	17	1.68
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	16	1.68
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	3	1.68
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	19	1.68
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD12	7	1.67
(1,869)	1:44:A:LEU:HA	1:44:A:LEU:HD13	15	1.67
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	15	1.67
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD11	2	1.67
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD13	3	1.67
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD13	4	1.67
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG11	16	1.67
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	14	1.65
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD21	19	1.65
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	3	1.65
(1,766)	1:49:A:VAL:HG11	1:46:A:GLN:HA	7	1.65
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	11	1.65
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	4	1.64
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG23	13	1.64
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	8	1.64
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG13	13	1.64
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	7	1.64
(1,766)	1:49:A:VAL:HG11	1:46:A:GLN:HA	12	1.63
(1,483)	1:62:A:THR:H	1:63:A:LEU:HD11	7	1.63
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	19	1.63
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	8	1.62
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	14	1.62
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	17	1.61
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	5	1.61
(1,839)	1:110:A:LEU:HD23	1:50:A:LEU:HD21	20	1.61
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	7	1.61
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	17	1.61
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	6	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	9	1.6
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD11	7	1.6
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	17	1.6
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD13	13	1.59
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	3	1.59
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	1	1.59
(1,453)	1:48:A:GLY:H	1:49:A:VAL:HG12	2	1.59
(1,7)	2:201:A:HEC:HBB3	1:96:A:VAL:HG11	19	1.59
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	13	1.58
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG12	17	1.58
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD12	4	1.58
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	7	1.57
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	14	1.57
(1,539)	1:89:A:ASP:H	1:35:A:ASN:HD22	8	1.57
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	20	1.56
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD13	4	1.56
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD11	17	1.56
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD12	18	1.56
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD11	7	1.55
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	8	1.55
(1,893)	1:26:A:VAL:HG13	1:27:A:PRO:HD3	13	1.55
(1,893)	1:26:A:VAL:HG13	1:27:A:PRO:HD3	20	1.55
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	10	1.55
(1,614)	1:118:A:LEU:H	1:119:A:VAL:HG21	17	1.55
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	9	1.55
(1,893)	1:26:A:VAL:HG12	1:27:A:PRO:HD3	18	1.54
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	9	1.53
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD11	20	1.53
(1,893)	1:26:A:VAL:HG11	1:27:A:PRO:HD3	6	1.52
(1,893)	1:26:A:VAL:HG11	1:27:A:PRO:HD3	14	1.52
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	6	1.52
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD11	8	1.52
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	7	1.52
(1,1097)	1:102:A:PRO:HB2	1:73:A:LEU:HD12	11	1.51
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	8	1.51
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	10	1.51
(1,1014)	1:63:A:LEU:H	1:63:A:LEU:HD13	3	1.51
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	1	1.51
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG22	18	1.51
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	8	1.51
(1,4)	1:118:A:LEU:HD21	2:201:A:HEC:HMB1	15	1.51
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	10	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD23	14	1.5
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG22	8	1.5
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	5	1.49
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	13	1.49
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD23	2	1.49
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	10	1.49
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD12	12	1.49
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD11	16	1.49
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG22	7	1.49
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	4	1.48
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	19	1.47
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG11	17	1.47
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD21	12	1.47
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	6	1.47
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	10	1.47
(1,1074)	1:81:A:VAL:HG11	1:64:A:ARG:HG2	11	1.46
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	20	1.46
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	15	1.46
(1,1074)	1:81:A:VAL:HG11	1:64:A:ARG:HG2	17	1.45
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	8	1.45
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	11	1.45
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	14	1.45
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	1	1.44
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD11	5	1.44
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	10	1.44
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	6	1.43
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	12	1.43
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	19	1.43
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	14	1.43
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	20	1.43
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	3	1.43
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG13	20	1.43
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	5	1.42
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	13	1.42
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD21	6	1.42
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	14	1.42
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	1	1.41
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG13	3	1.41
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG12	4	1.41
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	6	1.41
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	18	1.4
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	4	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	19	1.4
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	4	1.4
(1,892)	1:26:A:VAL:HG13	1:27:A:PRO:HD2	13	1.39
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG12	4	1.39
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	19	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	3	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG13	7	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	14	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	15	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	17	1.39
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	20	1.39
(1,697)	1:24:A:TRP:HB3	1:26:A:VAL:HG23	13	1.39
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG11	7	1.38
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	10	1.38
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	11	1.38
(1,766)	1:49:A:VAL:HG11	1:46:A:GLN:HA	18	1.38
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	20	1.37
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	20	1.37
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	1	1.37
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG13	12	1.37
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG13	13	1.37
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	1	1.36
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG12	11	1.36
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	9	1.36
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG13	18	1.36
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	2	1.36
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD13	17	1.36
(1,701)	1:50:A:LEU:HD23	1:110:A:LEU:HD11	14	1.36
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	6	1.35
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	8	1.35
(1,766)	1:49:A:VAL:HG11	1:46:A:GLN:HA	13	1.35
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD12	7	1.35
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD13	11	1.35
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	8	1.34
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG11	16	1.34
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	8	1.34
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	6	1.34
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	2	1.33
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG11	5	1.33
(1,768)	1:49:A:VAL:H	1:49:A:VAL:HG12	2	1.33
(1,766)	1:49:A:VAL:HG12	1:46:A:GLN:HA	16	1.33
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD21	15	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	14	1.31
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD13	15	1.31
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD13	12	1.31
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	5	1.31
(1,1091)	1:96:A:VAL:HG13	1:115:A:ILE:HG13	18	1.3
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG12	19	1.3
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	14	1.3
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	17	1.3
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	7	1.3
(1,839)	1:110:A:LEU:HD22	1:50:A:LEU:HD22	11	1.3
(1,772)	1:63:A:LEU:HB3	1:81:A:VAL:HG13	8	1.3
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD12	13	1.3
(1,1075)	1:63:A:LEU:HB2	1:81:A:VAL:HG12	17	1.29
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	13	1.29
(1,766)	1:49:A:VAL:HG13	1:46:A:GLN:HA	8	1.29
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD13	10	1.29
(1,744)	1:121:A:PHE:HA	1:44:A:LEU:HD11	11	1.29
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	6	1.29
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD11	12	1.29
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	16	1.28
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	2	1.28
(1,701)	1:50:A:LEU:HD21	1:110:A:LEU:HD12	15	1.28
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG11	17	1.28
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD13	11	1.28
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	3	1.27
(1,892)	1:26:A:VAL:HG13	1:27:A:PRO:HD2	20	1.27
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	13	1.27
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	1	1.27
(1,1041)	1:52:A:ALA:HB3	1:51:A:TYR:HB2	9	1.26
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD11	7	1.26
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	14	1.26
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG11	6	1.26
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	20	1.25
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	9	1.25
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	5	1.24
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	19	1.24
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	18	1.24
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD12	13	1.24
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD13	2	1.24
(1,1055)	1:63:A:LEU:HD21	1:125:A:ARG:HB2	3	1.23
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	3	1.23
(1,963)	1:118:A:LEU:HD23	1:51:A:TYR:HB3	5	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	16	1.23
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	11	1.22
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG13	14	1.22
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG12	8	1.22
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	20	1.22
(1,1041)	1:52:A:ALA:HB1	1:51:A:TYR:HB2	7	1.22
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG13	4	1.22
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG13	11	1.22
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	17	1.22
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG12	3	1.22
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	5	1.21
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	7	1.21
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	10	1.21
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	3	1.21
(1,892)	1:26:A:VAL:HG11	1:27:A:PRO:HD2	6	1.21
(1,1097)	1:102:A:PRO:HB2	1:73:A:LEU:HD12	1	1.2
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG11	6	1.2
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG11	20	1.2
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	12	1.2
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD21	20	1.2
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD12	17	1.2
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	3	1.2
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	9	1.2
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG13	3	1.19
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	4	1.19
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG11	13	1.19
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD22	12	1.19
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	1	1.19
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	2	1.19
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	18	1.19
(1,1097)	1:102:A:PRO:HB2	1:73:A:LEU:HD12	13	1.18
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG11	1	1.18
(1,1041)	1:52:A:ALA:HB2	1:51:A:TYR:HB2	15	1.18
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	18	1.18
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG13	17	1.18
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	10	1.18
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	2	1.17
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG13	8	1.17
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG12	17	1.17
(1,1073)	1:81:A:VAL:H	1:81:A:VAL:HG13	19	1.17
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD21	8	1.17
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	8	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	15	1.17
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	1	1.16
(1,972)	1:93:A:ALA:HA	1:96:A:VAL:HG21	8	1.16
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	10	1.16
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD12	15	1.16
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	13	1.16
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD13	13	1.16
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	10	1.15
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD22	14	1.15
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	19	1.15
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD23	10	1.15
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	19	1.15
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	20	1.15
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	11	1.14
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	3	1.14
(1,1074)	1:81:A:VAL:HG11	1:64:A:ARG:HG2	4	1.14
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	1	1.14
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG11	19	1.14
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	1	1.14
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	20	1.14
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD21	13	1.14
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	7	1.14
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	12	1.14
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	17	1.14
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	14	1.13
(1,1088)	1:106:A:PHE:HB2	1:96:A:VAL:HG12	19	1.13
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	19	1.13
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	1	1.13
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG11	11	1.13
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	4	1.13
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	16	1.13
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	19	1.12
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	16	1.12
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD22	10	1.12
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD23	17	1.12
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD13	20	1.12
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	17	1.11
(1,839)	1:110:A:LEU:HD21	1:50:A:LEU:HD22	10	1.11
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG11	3	1.11
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	12	1.11
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	15	1.11
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD12	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	9	1.11
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	11	1.11
(1,1056)	1:63:A:LEU:HD21	1:125:A:ARG:HB3	17	1.1
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	8	1.1
(1,539)	1:89:A:ASP:H	1:35:A:ASN:HD22	19	1.1
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	10	1.1
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	19	1.1
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG11	4	1.09
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	19	1.09
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	13	1.09
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	1	1.09
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	10	1.09
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD13	8	1.09
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	14	1.09
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	1	1.08
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG11	4	1.08
(1,972)	1:93:A:ALA:HA	1:96:A:VAL:HG21	5	1.08
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	7	1.08
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	13	1.08
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	4	1.08
(1,1091)	1:96:A:VAL:HG13	1:115:A:ILE:HG13	9	1.07
(1,1055)	1:63:A:LEU:HD21	1:125:A:ARG:HB2	7	1.07
(1,892)	1:26:A:VAL:HG11	1:27:A:PRO:HD2	14	1.07
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	7	1.07
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	18	1.07
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	6	1.07
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	5	1.07
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	4	1.07
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	12	1.06
(1,963)	1:118:A:LEU:HD23	1:51:A:TYR:HB3	17	1.06
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG13	8	1.06
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	10	1.06
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD22	11	1.06
(1,357)	1:124:A:ASP:H	1:44:A:LEU:HD11	13	1.06
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	7	1.05
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	10	1.05
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	17	1.05
(1,292)	1:49:A:VAL:H	1:50:A:LEU:HB3	6	1.05
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	5	1.05
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	6	1.04
(1,963)	1:118:A:LEU:HD23	1:51:A:TYR:HB3	1	1.04
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	7	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	15	1.04
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG11	6	1.04
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	3	1.04
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD23	15	1.04
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	18	1.04
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	1	1.03
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	4	1.03
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	20	1.02
(1,965)	1:56:A:VAL:HG21	1:56:A:VAL:HA	7	1.02
(1,931)	1:63:A:LEU:HD22	1:80:A:LEU:HB3	13	1.02
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	20	1.02
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	5	1.02
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	14	1.02
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD21	15	1.02
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	9	1.02
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	11	1.02
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	13	1.02
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	12	1.01
(1,1074)	1:81:A:VAL:HG13	1:64:A:ARG:HG2	7	1.01
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	18	1.01
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	15	1.01
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	17	1.01
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	20	1.01
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG12	3	1.0
(1,965)	1:56:A:VAL:HG22	1:56:A:VAL:HA	17	1.0
(1,963)	1:118:A:LEU:HD21	1:51:A:TYR:HB3	16	1.0
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG11	14	1.0
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	4	0.99
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	9	0.99
(1,430)	1:42:A:ARG:H	1:43:A:SER:HB3	11	0.99
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	14	0.99
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	3	0.98
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	7	0.98
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	1	0.98
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	14	0.98
(1,892)	1:26:A:VAL:HG12	1:27:A:PRO:HD2	4	0.98
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	20	0.98
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	6	0.98
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	14	0.98
(1,185)	1:30:A:GLU:H	1:26:A:VAL:HG11	14	0.98
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	8	0.98
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	16	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	14	0.97
(1,965)	1:56:A:VAL:HG21	1:56:A:VAL:HA	18	0.97
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	8	0.97
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	19	0.97
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	2	0.97
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	5	0.97
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG22	6	0.97
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	7	0.97
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	10	0.97
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	12	0.97
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	19	0.97
(1,892)	1:26:A:VAL:HG11	1:27:A:PRO:HD2	1	0.96
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	20	0.96
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG23	19	0.96
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	2	0.96
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	3	0.96
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	7	0.96
(1,870)	1:44:A:LEU:HD13	1:124:A:ASP:HB2	11	0.95
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD21	11	0.95
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	16	0.95
(1,1091)	1:96:A:VAL:HG11	1:115:A:ILE:HG13	16	0.94
(1,965)	1:56:A:VAL:HG23	1:56:A:VAL:HA	15	0.94
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	8	0.94
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	10	0.94
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	8	0.94
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	16	0.93
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	11	0.93
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	12	0.93
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	11	0.93
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	4	0.93
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	6	0.93
(1,1088)	1:106:A:PHE:HB2	1:96:A:VAL:HG12	8	0.92
(1,963)	1:118:A:LEU:HD23	1:51:A:TYR:HB3	4	0.92
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	18	0.92
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG12	8	0.92
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	7	0.92
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	1	0.92
(1,1074)	1:81:A:VAL:HG12	1:64:A:ARG:HG2	8	0.91
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG11	17	0.91
(1,972)	1:93:A:ALA:HA	1:96:A:VAL:HG22	19	0.91
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD23	7	0.91
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG23	13	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:37:A:ILE:H	1:37:A:ILE:HG13	14	0.91
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	10	0.9
(1,518)	1:80:A:LEU:H	1:81:A:VAL:HG12	5	0.9
(1,457)	1:52:A:ALA:H	1:118:A:LEU:HD21	15	0.9
(1,430)	1:42:A:ARG:H	1:43:A:SER:HB3	2	0.9
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	1	0.89
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	8	0.89
(1,963)	1:118:A:LEU:HD22	1:51:A:TYR:HB3	9	0.89
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	13	0.89
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD22	13	0.88
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	5	0.88
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	8	0.87
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	1	0.87
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	5	0.87
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	17	0.87
(1,800)	1:96:A:VAL:HG13	1:103:A:MET:HE2	5	0.86
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	20	0.86
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	10	0.86
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	20	0.86
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	9	0.86
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	20	0.85
(1,602)	1:116:A:TRP:H	1:112:A:GLU:HB2	11	0.85
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	15	0.85
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	4	0.84
(1,1088)	1:106:A:PHE:HB2	1:96:A:VAL:HG12	5	0.84
(1,843)	1:73:A:LEU:HD13	1:70:A:ALA:HB3	10	0.84
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	14	0.84
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD22	2	0.84
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	8	0.84
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	6	0.84
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	10	0.84
(1,701)	1:50:A:LEU:HD22	1:110:A:LEU:HD13	10	0.83
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	18	0.83
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	12	0.83
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	16	0.82
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	2	0.82
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	9	0.82
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	17	0.82
(1,1066)	1:73:A:LEU:HD12	1:102:A:PRO:HB3	11	0.81
(1,1040)	1:118:A:LEU:HD21	1:51:A:TYR:HB2	11	0.81
(1,870)	1:44:A:LEU:HD13	1:124:A:ASP:HB2	20	0.81
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	4	0.81
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	7	0.81
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	13	0.81
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	14	0.81
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	20	0.81
(1,282)	1:119:A:VAL:H	1:119:A:VAL:HG21	17	0.81
(1,1066)	1:73:A:LEU:HD12	1:102:A:PRO:HB3	1	0.8
(1,879)	1:78:A:ALA:HB2	1:83:A:HIS:HB3	5	0.8
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD22	4	0.8
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	3	0.8
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	11	0.8
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	13	0.8
(1,800)	1:96:A:VAL:HG13	1:103:A:MET:HE2	8	0.79
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	1	0.79
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	5	0.79
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	13	0.79
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	12	0.79
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	6	0.79
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	17	0.78
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	9	0.78
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	7	0.78
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	8	0.78
(1,1091)	1:96:A:VAL:HG13	1:115:A:ILE:HG13	13	0.77
(1,680)	1:116:A:TRP:HE1	1:112:A:GLU:HB2	13	0.77
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	11	0.77
(1,430)	1:42:A:ARG:H	1:43:A:SER:HB3	1	0.77
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	4	0.77
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	15	0.77
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD11	18	0.77
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	14	0.77
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	14	0.76
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	18	0.76
(1,459)	1:54:A:HIS:H	1:50:A:LEU:HD22	9	0.76
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	6	0.76
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD12	4	0.75
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	19	0.75
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	5	0.75
(1,1133)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	3	0.74
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD12	3	0.74
(1,865)	1:96:A:VAL:H	1:96:A:VAL:HG23	5	0.74
(1,488)	1:64:A:ARG:H	1:81:A:VAL:HG13	7	0.74
(1,434)	1:42:A:ARG:H	1:44:A:LEU:HD23	11	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	4	0.73
(1,1133)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	13	0.73
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG21	1	0.73
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	9	0.73
(1,430)	1:42:A:ARG:H	1:43:A:SER:HB3	14	0.73
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	16	0.73
(1,1133)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	7	0.72
(1,1133)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	17	0.72
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD11	13	0.72
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	6	0.72
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	8	0.72
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	13	0.72
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	9	0.72
(1,1056)	1:63:A:LEU:HD21	1:125:A:ARG:HB3	4	0.71
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	6	0.71
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD13	7	0.71
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG21	8	0.71
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	20	0.71
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	1	0.71
(1,1040)	1:118:A:LEU:HD22	1:51:A:TYR:HB2	10	0.7
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG12	19	0.7
(1,865)	1:96:A:VAL:H	1:96:A:VAL:HG23	8	0.7
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	6	0.7
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG23	4	0.7
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	14	0.7
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	16	0.7
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	7	0.7
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	5	0.69
(1,1091)	1:96:A:VAL:HG12	1:115:A:ILE:HG13	15	0.69
(1,814)	1:50:A:LEU:HG	1:110:A:LEU:HD21	3	0.69
(1,602)	1:116:A:TRP:H	1:112:A:GLU:HB2	13	0.69
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	8	0.69
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	10	0.69
(1,409)	1:30:A:GLU:H	1:32:A:HIS:HB3	19	0.69
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	1	0.69
(1,1055)	1:63:A:LEU:HD21	1:125:A:ARG:HB2	17	0.68
(1,1040)	1:118:A:LEU:HD23	1:51:A:TYR:HB2	15	0.68
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD23	9	0.68
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	10	0.68
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	14	0.68
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG23	1	0.68
(1,865)	1:96:A:VAL:H	1:96:A:VAL:HG21	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	1	0.67
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	6	0.67
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	5	0.66
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	11	0.66
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	7	0.66
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	19	0.66
(1,450)	1:47:A:GLY:H	1:50:A:LEU:HB3	3	0.66
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	16	0.66
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	4	0.65
(1,1066)	1:73:A:LEU:HD12	1:102:A:PRO:HB3	13	0.65
(1,875)	1:63:A:LEU:HA	1:63:A:LEU:HD13	17	0.65
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	16	0.65
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	18	0.65
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	6	0.65
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG21	18	0.65
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	2	0.65
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	13	0.65
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	6	0.64
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG22	18	0.64
(1,870)	1:44:A:LEU:HD12	1:124:A:ASP:HB2	15	0.64
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	6	0.64
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	14	0.64
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	13	0.63
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	14	0.63
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	13	0.63
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	2	0.63
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	7	0.63
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	18	0.63
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	7	0.63
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	11	0.63
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	4	0.62
(1,1056)	1:63:A:LEU:HD23	1:125:A:ARG:HB3	13	0.62
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG13	20	0.62
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB2	7	0.62
(1,539)	1:89:A:ASP:H	1:35:A:ASN:HD22	14	0.62
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG21	7	0.62
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	4	0.62
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG12	11	0.61
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG22	3	0.61
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	17	0.61
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	17	0.6
(1,870)	1:44:A:LEU:HD11	1:124:A:ASP:HB2	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:44:A:LEU:HD12	1:124:A:ASP:HB2	10	0.6
(1,870)	1:44:A:LEU:HD11	1:124:A:ASP:HB2	13	0.6
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	1	0.6
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	8	0.6
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	13	0.6
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	19	0.6
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD12	15	0.59
(1,1055)	1:63:A:LEU:HD23	1:125:A:ARG:HB2	13	0.58
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	3	0.58
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	12	0.58
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	15	0.58
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	11	0.58
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	2	0.58
(1,190)	1:26:A:VAL:H	1:26:A:VAL:HG21	9	0.58
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD12	8	0.58
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	3	0.57
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	10	0.57
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	3	0.57
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	2	0.57
(1,870)	1:44:A:LEU:HD11	1:124:A:ASP:HB2	12	0.56
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	9	0.56
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	1	0.56
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	3	0.56
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	5	0.56
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	8	0.56
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	12	0.56
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	19	0.56
(1,791)	1:44:A:LEU:HD21	1:44:A:LEU:HB2	7	0.56
(1,791)	1:44:A:LEU:HD21	1:44:A:LEU:HB2	11	0.56
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	12	0.56
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	6	0.56
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	17	0.56
(1,870)	1:44:A:LEU:HD12	1:124:A:ASP:HB2	17	0.55
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	2	0.55
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	4	0.55
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	6	0.55
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	7	0.55
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	9	0.55
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	11	0.55
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	13	0.55
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	14	0.55
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	16	0.55
(1,826)	1:37:A:ILE:HG23	1:37:A:ILE:HG12	18	0.55
(1,791)	1:44:A:LEU:HD23	1:44:A:LEU:HB2	12	0.55
(1,791)	1:44:A:LEU:HD22	1:44:A:LEU:HB2	15	0.55
(1,791)	1:44:A:LEU:HD21	1:44:A:LEU:HB2	17	0.55
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	4	0.55
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	1	0.55
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	1	0.54
(1,870)	1:44:A:LEU:HD13	1:124:A:ASP:HB2	8	0.54
(1,826)	1:37:A:ILE:HG22	1:37:A:ILE:HG12	17	0.54
(1,826)	1:37:A:ILE:HG21	1:37:A:ILE:HG12	20	0.54
(1,791)	1:44:A:LEU:HD22	1:44:A:LEU:HB2	8	0.54
(1,791)	1:44:A:LEU:HD22	1:44:A:LEU:HB2	13	0.54
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	7	0.53
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG13	7	0.53
(1,791)	1:44:A:LEU:HD23	1:44:A:LEU:HB2	10	0.53
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	18	0.53
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	19	0.52
(1,1055)	1:63:A:LEU:HD21	1:125:A:ARG:HB2	4	0.52
(1,928)	1:63:A:LEU:HD22	1:80:A:LEU:HB2	13	0.52
(1,791)	1:44:A:LEU:HD22	1:44:A:LEU:HB2	20	0.52
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	5	0.52
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	1	0.51
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	17	0.51
(1,879)	1:78:A:ALA:HB3	1:83:A:HIS:HB3	20	0.51
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	1	0.51
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	4	0.51
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	16	0.51
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	12	0.51
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	7	0.51
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG13	1	0.5
(1,879)	1:78:A:ALA:HB2	1:83:A:HIS:HB3	15	0.5
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	17	0.5
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	5	0.5
(1,516)	1:79:A:ASP:H	1:82:A:GLU:HB2	11	0.5
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	6	0.5
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	5	0.5
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	7	0.49
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	7	0.49
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	19	0.49
(1,704)	1:50:A:LEU:HD11	1:50:A:LEU:H	5	0.49
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	16	0.48
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	7	0.48
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB1	13	0.48
(1,702)	1:50:A:LEU:HD11	1:46:A:GLN:HG3	3	0.48
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	6	0.48
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	17	0.48
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	11	0.47
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	8	0.47
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	14	0.46
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	19	0.46
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	1	0.46
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB1	11	0.46
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	3	0.46
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	4	0.46
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	3	0.46
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	11	0.46
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	15	0.46
(1,1052)	1:61:A:GLU:HG3	1:56:A:VAL:HG22	18	0.45
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	15	0.45
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	13	0.45
(1,880)	1:115:A:ILE:HD13	1:107:A:GLY:HA3	6	0.44
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB3	6	0.44
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	16	0.44
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	17	0.44
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	16	0.44
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	20	0.44
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	14	0.44
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	19	0.44
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	20	0.44
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	15	0.43
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD21	3	0.43
(1,452)	1:48:A:GLY:H	1:50:A:LEU:HB3	5	0.43
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	4	0.43
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	19	0.43
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	18	0.42
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB2	3	0.42
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	11	0.42
(1,269)	1:46:A:GLN:HE22	1:50:A:LEU:HD13	5	0.42
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD11	18	0.42
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	18	0.42
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	8	0.41
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	15	0.41
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG11	4	0.41
(1,880)	1:115:A:ILE:HD12	1:107:A:GLY:HA3	15	0.41
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	1	0.41
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB3	10	0.41
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	15	0.41
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	4	0.41
(1,1120)	1:115:A:ILE:HD13	1:97:A:ARG:HD2	2	0.4
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	10	0.4
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	2	0.4
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	18	0.4
(1,880)	1:115:A:ILE:HD12	1:107:A:GLY:HA3	3	0.4
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	14	0.4
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	17	0.4
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB2	17	0.4
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG11	17	0.4
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	12	0.4
(1,1052)	1:61:A:GLU:HG3	1:56:A:VAL:HG21	1	0.39
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG12	8	0.39
(1,880)	1:115:A:ILE:HD13	1:107:A:GLY:HA3	14	0.39
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	4	0.39
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	13	0.39
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	13	0.39
(1,403)	1:25:A:GLU:H	1:100:A:ARG:HD2	9	0.39
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	13	0.38
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	3	0.38
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	17	0.38
(1,502)	1:70:A:ALA:H	1:73:A:LEU:HD11	6	0.38
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	18	0.38
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	8	0.38
(1,1031)	1:41:A:ALA:HB1	1:40:A:ASP:HB3	15	0.37
(1,879)	1:78:A:ALA:HB2	1:83:A:HIS:HB3	2	0.37
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	2	0.37
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	4	0.37
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG23	13	0.37
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	8	0.37
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	17	0.37
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	16	0.37
(1,1136)	1:26:A:VAL:HG13	1:31:A:ILE:HG13	13	0.36
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	19	0.36
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	13	0.36
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	2	0.36
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	9	0.36
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	12	0.36
(1,402)	1:24:A:TRP:HE1	1:23:A:GLY:HA3	13	0.36
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	9	0.35
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	18	0.35
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	13	0.35
(1,979)	1:64:A:ARG:HD3	1:81:A:VAL:HG12	3	0.35
(1,800)	1:96:A:VAL:HG13	1:103:A:MET:HE2	19	0.35
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	14	0.35
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	10	0.35
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB1	9	0.35
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG12	6	0.34
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	8	0.34
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	16	0.34
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	1	0.34
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	15	0.34
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	20	0.34
(1,402)	1:24:A:TRP:HE1	1:23:A:GLY:HA3	15	0.34
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	10	0.34
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	19	0.34
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG12	1	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG11	13	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG12	14	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	18	0.33
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	13	0.33
(1,843)	1:73:A:LEU:HD12	1:70:A:ALA:HB3	3	0.33
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	6	0.33
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	10	0.33
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG23	18	0.33
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	6	0.33
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	1	0.33
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	12	0.33
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	5	0.33
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	4	0.32
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	7	0.32
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG11	20	0.32
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG11	11	0.32
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	10	0.32
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	8	0.32
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG11	2	0.32
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	5	0.32
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	20	0.32
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	3	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	2	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	6	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	8	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	9	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	11	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	12	0.32
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	16	0.32
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	3	0.31
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	12	0.31
(1,923)	1:93:A:ALA:HB1	1:115:A:ILE:HG23	12	0.31
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD23	4	0.31
(1,580)	1:106:A:PHE:H	1:96:A:VAL:HG12	19	0.31
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	14	0.31
(1,402)	1:24:A:TRP:HE1	1:23:A:GLY:HA3	14	0.31
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	13	0.31
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	14	0.31
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	17	0.31
(1,1135)	1:26:A:VAL:HA	1:26:A:VAL:HG13	9	0.3
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	6	0.3
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	18	0.3
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD21	7	0.3
(1,785)	1:51:A:TYR:HA	1:55:A:CYS:HB3	1	0.3
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	18	0.3
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	8	0.3
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG12	3	0.3
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG23	7	0.3
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	10	0.3
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	3	0.3
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	7	0.3
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	15	0.3
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	18	0.3
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	20	0.3
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	11	0.29
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	16	0.29
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	5	0.29
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	17	0.29
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	3	0.29
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB3	2	0.29
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:50:A:LEU:HD11	1:50:A:LEU:H	13	0.29
(1,667)	1:96:A:VAL:H	1:99:A:GLY:HA3	20	0.29
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	16	0.29
(1,580)	1:106:A:PHE:H	1:96:A:VAL:HG12	8	0.29
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	3	0.29
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	13	0.29
(1,403)	1:25:A:GLU:H	1:100:A:ARG:HD2	10	0.29
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	4	0.29
(1,858)	1:89:A:ASP:HB2	1:119:A:VAL:HG12	20	0.28
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	10	0.28
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	13	0.28
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	7	0.28
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	16	0.28
(1,110)	1:46:A:GLN:HE21	1:50:A:LEU:HD13	5	0.28
(1,109)	1:46:A:GLN:HE21	1:50:A:LEU:HB3	3	0.28
(1,17)	1:116:A:TRP:H	1:116:A:TRP:HB3	1	0.28
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	20	0.27
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	15	0.27
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	18	0.27
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	2	0.27
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	12	0.27
(1,709)	1:81:A:VAL:HG22	1:129:A:ALA:HB3	19	0.27
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	15	0.27
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	16	0.27
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	18	0.27
(1,502)	1:70:A:ALA:H	1:73:A:LEU:HD13	10	0.27
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	10	0.27
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	9	0.26
(1,782)	1:125:A:ARG:HD2	1:125:A:ARG:HA	12	0.26
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	5	0.26
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	19	0.26
(1,428)	1:40:A:ASP:H	1:41:A:ALA:HB2	1	0.26
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	4	0.26
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	6	0.26
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	11	0.26
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	13	0.25
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	15	0.25
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	9	0.25
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	20	0.25
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	16	0.25
(1,877)	1:70:A:ALA:HA	1:73:A:LEU:HD11	6	0.25
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	14	0.25
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	1	0.25
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	9	0.25
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG12	9	0.25
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	20	0.25
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	15	0.25
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	15	0.25
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	4	0.25
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG13	14	0.25
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	9	0.25
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	1	0.25
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD11	18	0.25
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	15	0.25
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	14	0.24
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	6	0.24
(1,843)	1:73:A:LEU:HD13	1:70:A:ALA:HB3	7	0.24
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	5	0.24
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	19	0.24
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	17	0.24
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG22	17	0.24
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	18	0.24
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	6	0.24
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	12	0.24
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	5	0.24
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	2	0.23
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	17	0.23
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	10	0.23
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD23	2	0.23
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	15	0.23
(1,879)	1:78:A:ALA:HB1	1:83:A:HIS:HB3	3	0.23
(1,843)	1:73:A:LEU:HD13	1:70:A:ALA:HB3	8	0.23
(1,843)	1:73:A:LEU:HD12	1:70:A:ALA:HB3	19	0.23
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	7	0.23
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	2	0.23
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG11	6	0.23
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	15	0.23
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	15	0.23
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	12	0.23
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD23	14	0.22
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD21	20	0.22
(1,893)	1:26:A:VAL:HG11	1:27:A:PRO:HD3	19	0.22
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:125:A:ARG:HD2	1:125:A:ARG:HA	15	0.22
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	10	0.22
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	16	0.22
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	4	0.22
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	2	0.22
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	12	0.21
(1,1102)	1:102:A:PRO:HG2	1:73:A:LEU:HB2	20	0.21
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG12	14	0.21
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG21	14	0.21
(1,1022)	1:36:A:PRO:HD2	1:35:A:ASN:HB2	11	0.21
(1,836)	1:110:A:LEU:HD21	1:106:A:PHE:HB3	7	0.21
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	8	0.21
(1,836)	1:110:A:LEU:HD21	1:106:A:PHE:HB3	20	0.21
(1,785)	1:51:A:TYR:HA	1:55:A:CYS:HB3	3	0.21
(1,709)	1:81:A:VAL:HG22	1:129:A:ALA:HB3	18	0.21
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	11	0.21
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	3	0.21
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	13	0.21
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG22	4	0.21
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD13	13	0.21
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	9	0.21
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	16	0.2
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	4	0.2
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	11	0.2
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	18	0.2
(1,743)	1:121:A:PHE:HA	1:124:A:ASP:HB2	8	0.2
(1,709)	1:81:A:VAL:HG21	1:129:A:ALA:HB1	4	0.2
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	11	0.2
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	4	0.2
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG12	11	0.2
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG12	19	0.2
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	2	0.2
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD12	1	0.2
(1,78)	1:37:A:ILE:H	1:36:A:PRO:HD3	6	0.2
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	19	0.2
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG22	7	0.19
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	19	0.19
(1,952)	1:109:A:ALA:HB1	1:110:A:LEU:HD21	5	0.19
(1,918)	1:114:A:ASP:HB3	1:50:A:LEU:HD22	10	0.19
(1,879)	1:78:A:ALA:HB3	1:83:A:HIS:HB3	19	0.19
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	5	0.19
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	5	0.19
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	6	0.19
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	7	0.19
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	1	0.19
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	8	0.19
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	14	0.19
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	19	0.19
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	2	0.19
(1,77)	1:37:A:ILE:H	1:116:A:TRP:HB2	9	0.19
(1,26)	1:99:A:GLY:H	1:95:A:ARG:HB3	2	0.19
(1,843)	1:73:A:LEU:HD13	1:70:A:ALA:HB3	18	0.18
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	6	0.18
(1,704)	1:50:A:LEU:HD11	1:50:A:LEU:H	2	0.18
(1,681)	1:116:A:TRP:HE1	1:112:A:GLU:HG3	14	0.18
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	9	0.18
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	16	0.18
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	16	0.18
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD12	9	0.18
(1,411)	1:31:A:ILE:H	1:32:A:HIS:HB3	19	0.18
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	2	0.18
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	5	0.18
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	6	0.18
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	7	0.18
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	15	0.18
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	13	0.18
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	3	0.18
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	9	0.18
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	10	0.18
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	12	0.18
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	1	0.18
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	3	0.17
(1,898)	1:122:A:MET:HA	1:63:A:LEU:HD21	17	0.17
(1,893)	1:26:A:VAL:HG13	1:27:A:PRO:HD3	2	0.17
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	9	0.17
(1,871)	1:44:A:LEU:HD11	1:120:A:ASN:HB2	16	0.17
(1,844)	1:73:A:LEU:HB3	1:73:A:LEU:HD12	13	0.17
(1,836)	1:110:A:LEU:HD21	1:106:A:PHE:HB3	4	0.17
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	8	0.17
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	14	0.17
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG12	14	0.17
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	13	0.17
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	20	0.17
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	20	0.17
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD11	15	0.17
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	4	0.17
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	9	0.17
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	10	0.17
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	18	0.17
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	20	0.17
(1,141)	1:97:A:ARG:H	1:97:A:ARG:HB3	17	0.17
(1,78)	1:37:A:ILE:H	1:36:A:PRO:HD3	4	0.17
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	5	0.17
(1,1060)	1:64:A:ARG:HD2	1:81:A:VAL:HG13	7	0.16
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	1	0.16
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	16	0.16
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	17	0.16
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	5	0.16
(1,660)	1:69:A:ASP:H	1:77:A:VAL:HG11	8	0.16
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	2	0.16
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	14	0.16
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	17	0.16
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG11	8	0.16
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	11	0.16
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	2	0.16
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD12	4	0.16
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	16	0.16
(1,162)	1:83:A:HIS:H	1:82:A:GLU:HB2	11	0.16
(1,58)	1:60:A:GLY:H	1:59:A:HIS:H	18	0.16
(1,53)	1:41:A:ALA:H	1:40:A:ASP:HB3	14	0.16
(1,1128)	1:126:A:ALA:HB2	1:85:A:PRO:HD2	3	0.15
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	8	0.15
(1,844)	1:73:A:LEU:HB3	1:73:A:LEU:HD12	1	0.15
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	1	0.15
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	16	0.15
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB1	13	0.15
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD11	16	0.15
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	12	0.15
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	17	0.15
(1,199)	1:65:A:GLY:H	1:60:A:GLY:HA2	1	0.15
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	6	0.15
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	15	0.14
(1,844)	1:73:A:LEU:HB3	1:73:A:LEU:HD12	11	0.14
(1,843)	1:73:A:LEU:HD11	1:70:A:ALA:HB3	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:50:A:LEU:HD11	1:50:A:LEU:H	11	0.14
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG13	19	0.14
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG22	3	0.14
(1,602)	1:116:A:TRP:H	1:112:A:GLU:HB2	3	0.14
(1,446)	1:46:A:GLN:HE22	1:50:A:LEU:HB3	17	0.14
(1,58)	1:60:A:GLY:H	1:59:A:HIS:H	19	0.14
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	3	0.14
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	4	0.14
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	20	0.14
(1,1108)	1:110:A:LEU:HB3	1:114:A:ASP:HB2	12	0.13
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG21	15	0.13
(1,1031)	1:41:A:ALA:HB3	1:40:A:ASP:HB3	11	0.13
(1,1031)	1:41:A:ALA:HB1	1:40:A:ASP:HB3	12	0.13
(1,952)	1:109:A:ALA:HB2	1:110:A:LEU:HD21	6	0.13
(1,709)	1:81:A:VAL:HG23	1:129:A:ALA:HB1	9	0.13
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	1	0.13
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	3	0.13
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	12	0.13
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	15	0.13
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB1	15	0.13
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG11	13	0.13
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	1	0.13
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	15	0.13
(1,540)	1:89:A:ASP:H	1:119:A:VAL:HG11	5	0.13
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	2	0.13
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	8	0.13
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	18	0.13
(1,1054)	1:63:A:LEU:HB3	1:80:A:LEU:HB2	13	0.12
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG21	4	0.12
(1,1048)	1:61:A:GLU:HG2	1:56:A:VAL:HG23	17	0.12
(1,880)	1:115:A:ILE:HD11	1:107:A:GLY:HA3	11	0.12
(1,871)	1:44:A:LEU:HD13	1:120:A:ASN:HB2	18	0.12
(1,871)	1:44:A:LEU:HD12	1:120:A:ASN:HB2	19	0.12
(1,836)	1:110:A:LEU:HD22	1:106:A:PHE:HB3	15	0.12
(1,785)	1:51:A:TYR:HA	1:55:A:CYS:HB3	18	0.12
(1,704)	1:50:A:LEU:HD12	1:50:A:LEU:H	19	0.12
(1,684)	1:77:A:VAL:H	1:76:A:PRO:HB3	10	0.12
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	19	0.12
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	20	0.12
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	20	0.12
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	10	0.12
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG21	1	0.12
(1,594)	1:112:A:GLU:H	1:115:A:ILE:HG12	14	0.12
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	1	0.12
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD11	7	0.12
(1,402)	1:24:A:TRP:HE1	1:23:A:GLY:HA3	16	0.12
(1,372)	1:112:A:GLU:H	1:112:A:GLU:HB3	3	0.12
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	12	0.12
(1,1116)	1:113:A:ARG:HA	1:37:A:ILE:HG12	9	0.11
(1,1115)	1:112:A:GLU:HA	1:115:A:ILE:HG12	20	0.11
(1,1054)	1:63:A:LEU:HB3	1:80:A:LEU:HB2	5	0.11
(1,1031)	1:41:A:ALA:HB2	1:40:A:ASP:HB3	6	0.11
(1,952)	1:109:A:ALA:HB1	1:110:A:LEU:HD23	12	0.11
(1,836)	1:110:A:LEU:HD23	1:106:A:PHE:HB3	19	0.11
(1,785)	1:51:A:TYR:HA	1:55:A:CYS:HB3	7	0.11
(1,704)	1:50:A:LEU:HD13	1:50:A:LEU:H	15	0.11
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	4	0.11
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB3	10	0.11
(1,651)	1:49:A:VAL:H	1:52:A:ALA:HB1	11	0.11
(1,625)	1:43:A:SER:H	1:120:A:ASN:HD22	18	0.11
(1,604)	1:116:A:TRP:H	1:37:A:ILE:HG22	14	0.11
(1,494)	1:66:A:ASP:H	1:67:A:GLY:HA2	17	0.11
(1,448)	1:46:A:GLN:HE21	1:46:A:GLN:HB3	17	0.11
(1,410)	1:30:A:GLU:H	1:31:A:ILE:HD11	17	0.11
(1,309)	1:74:A:ASP:H	1:73:A:LEU:HB2	4	0.11
(1,309)	1:74:A:ASP:H	1:73:A:LEU:HB2	5	0.11
(1,197)	1:111:A:ASP:H	1:110:A:LEU:HD21	17	0.11
(1,53)	1:41:A:ALA:H	1:40:A:ASP:HB3	3	0.11
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	10	0.11
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	17	0.11
(1,47)	1:54:A:HIS:H	1:54:A:HIS:HB3	19	0.11
(1,1054)	1:63:A:LEU:HB3	1:80:A:LEU:HB2	3	0.1
(1,1028)	1:37:A:ILE:HG23	1:116:A:TRP:HB2	18	0.1
(1,817)	1:53:A:GLU:HG3	1:53:A:GLU:HA	8	0.1
(1,657)	1:64:A:ARG:H	1:64:A:ARG:HB3	8	0.1
(1,631)	1:123:A:ARG:H	1:119:A:VAL:HG13	11	0.1
(1,627)	1:121:A:PHE:H	1:122:A:MET:HB3	4	0.1
(1,602)	1:116:A:TRP:H	1:112:A:GLU:HB2	6	0.1
(1,522)	1:81:A:VAL:H	1:63:A:LEU:HD13	15	0.1

10 Dihedral-angle violation analysis (i)

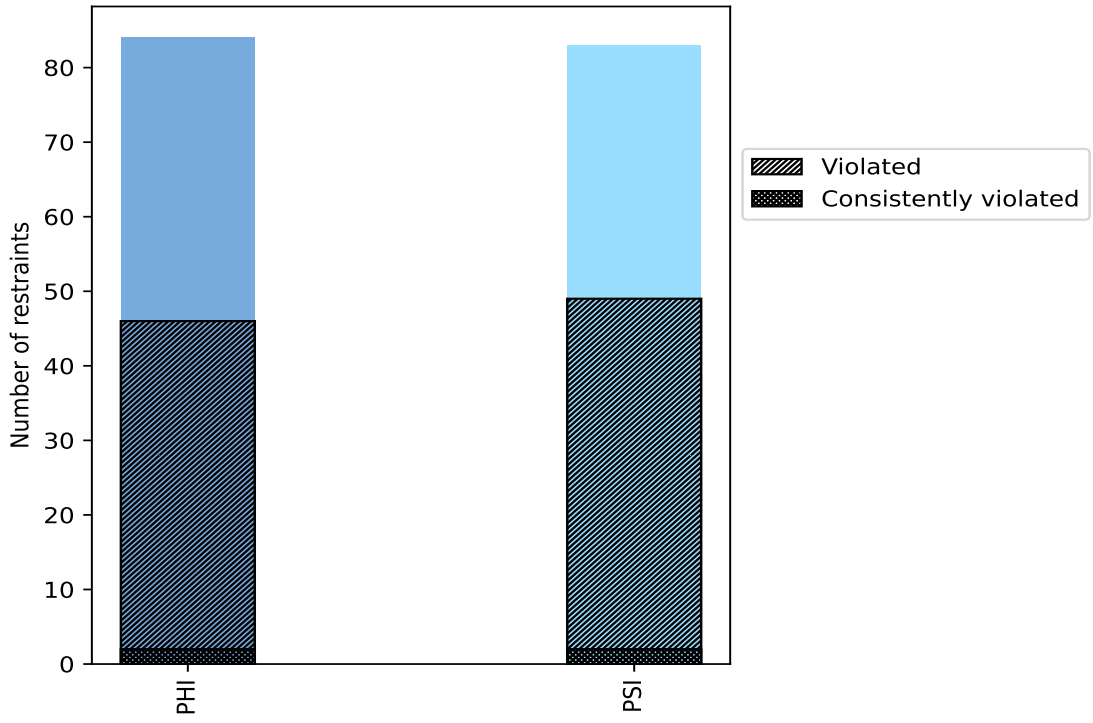
10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	84	50.3	46	54.8	27.5	2	2.4	1.2
PSI	83	49.7	49	59.0	29.3	2	2.4	1.2
Total	167	100.0	95	56.9	56.9	4	2.4	2.4

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



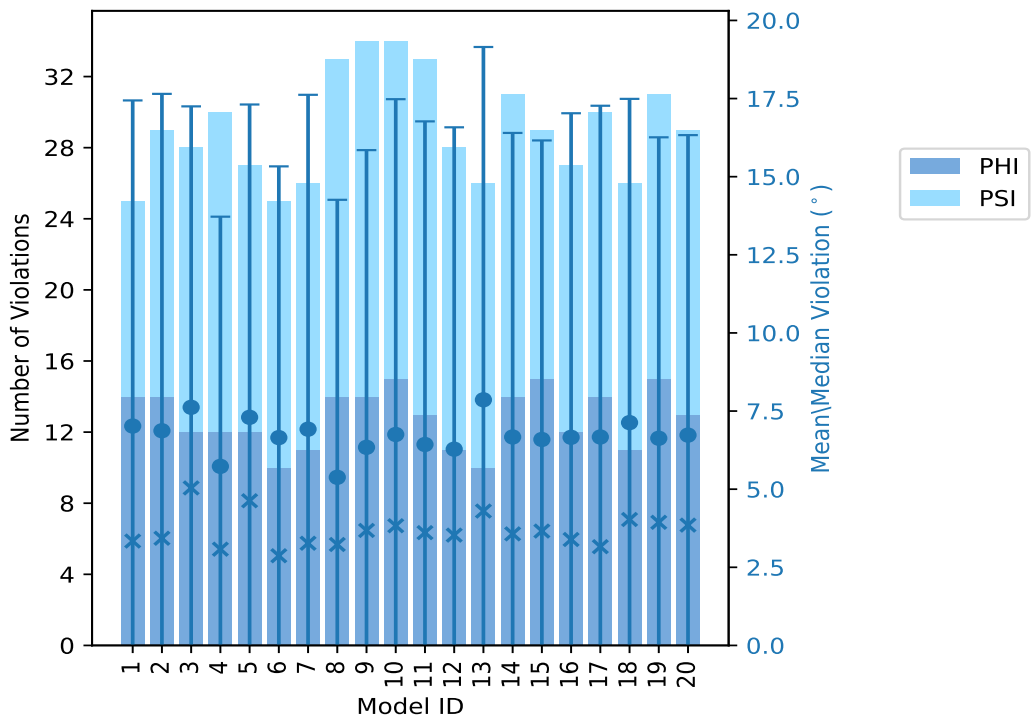
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	14	11	25	7.02	50.68	10.42	3.34
2	14	15	29	6.87	57.46	10.78	3.43
3	12	16	28	7.62	48.97	9.63	5.04
4	12	18	30	5.73	42.15	7.99	3.08
5	12	15	27	7.3	52.19	10.01	4.63
6	10	15	25	6.65	42.63	8.68	2.87
7	11	15	26	6.92	54.01	10.7	3.27
8	14	19	33	5.38	49.67	8.88	3.23
9	14	20	34	6.34	53.68	9.51	3.68
10	15	19	34	6.75	62.5	10.73	3.83
11	13	20	33	6.43	57.89	10.34	3.61
12	11	17	28	6.28	53.54	10.3	3.53
13	10	16	26	7.86	57.36	11.29	4.3
14	14	17	31	6.67	52.53	9.73	3.57
15	15	14	29	6.59	51.41	9.57	3.66
16	12	15	27	6.66	53.22	10.37	3.39
17	14	16	30	6.67	56.09	10.6	3.16
18	11	15	26	7.13	51.55	10.36	4.03
19	15	16	31	6.63	53.26	9.63	3.94
20	13	16	29	6.73	50.78	9.6	3.85

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
11	11	22	1	5.0
9	6	15	2	10.0
5	2	7	3	15.0
4	2	6	4	20.0
0	6	6	5	25.0
3	4	7	6	30.0
4	3	7	7	35.0
1	0	1	8	40.0
1	2	3	9	45.0
0	2	2	10	50.0
1	1	2	11	55.0

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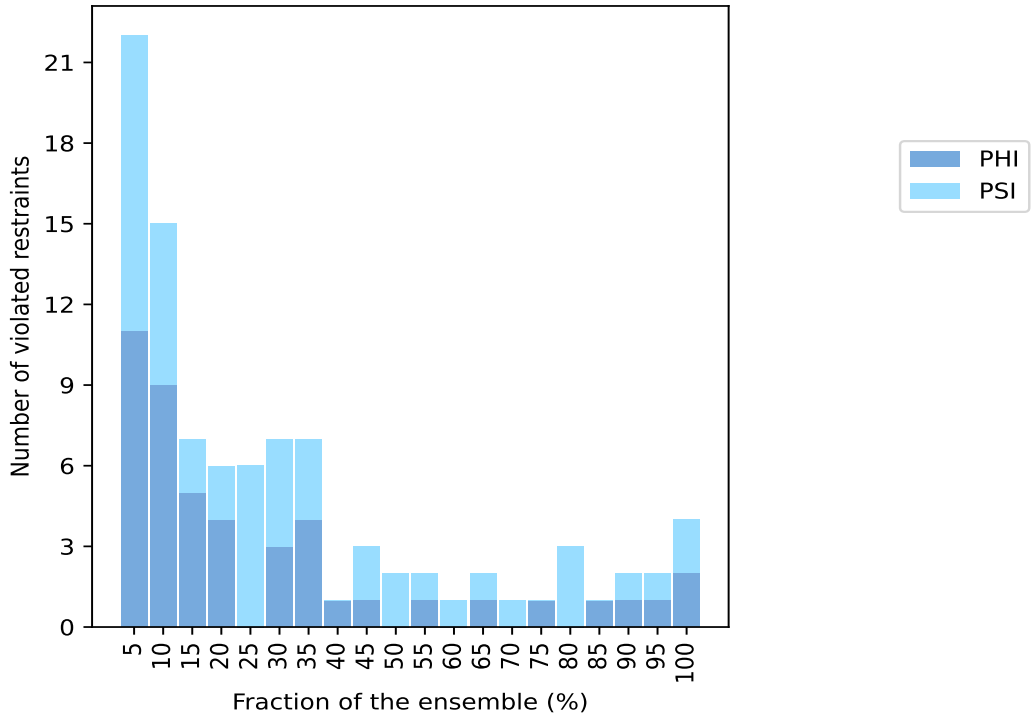
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	1	1	12	60.0
1	1	2	13	65.0
0	1	1	14	70.0
1	0	1	15	75.0
0	3	3	16	80.0
1	0	1	17	85.0
1	1	2	18	90.0
1	1	2	19	95.0
2	2	4	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)

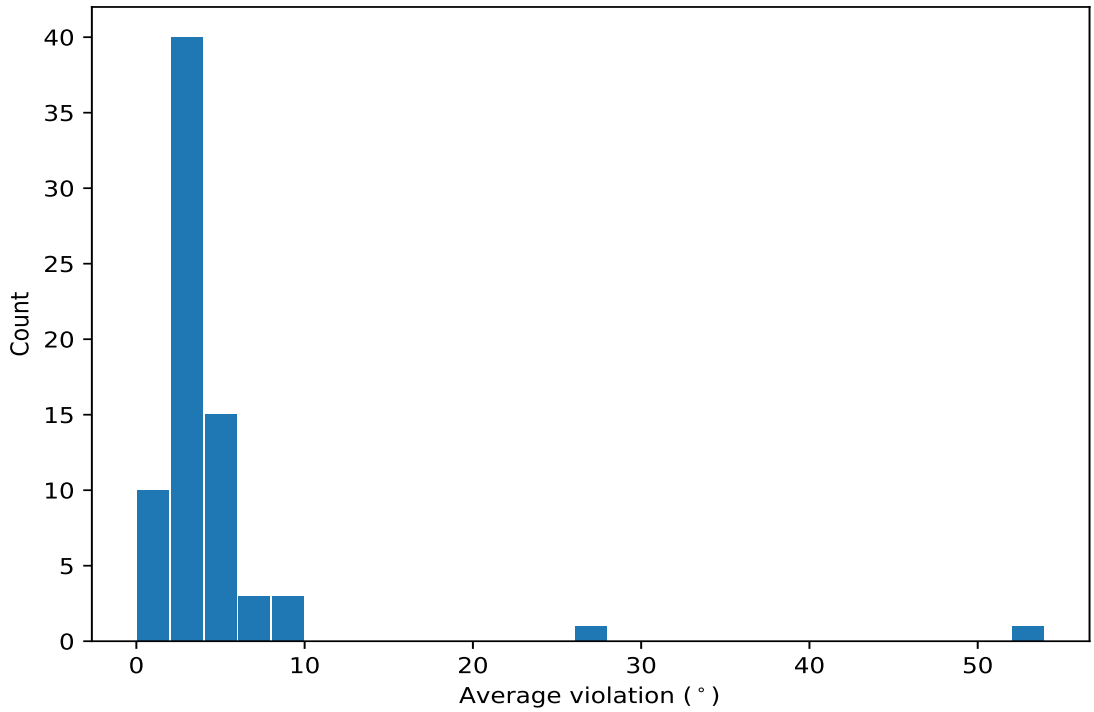


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	20	52.58	4.63	52.88
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	20	26.16	2.05	26.57
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	20	9.51	2.92	9.37
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	20	9.38	3.22	9.85
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	19	4.89	1.93	5.37
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	19	3.47	1.09	3.44
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	18	7.1	3.31	6.38
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	18	3.77	1.4	3.42
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	17	5.65	2.32	5.89
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	16	8.1	3.52	8.22
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	16	4.13	1.88	3.68
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	16	3.94	2.15	3.7
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	15	4.55	2.72	3.34
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	14	4.12	1.6	4.1
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	13	4.62	2.32	5.46
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	13	4.56	2.33	5.23
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	12	3.24	1.86	2.63
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	11	4.16	1.82	3.94
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	11	3.94	1.58	4.51
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	10	3.93	2.52	2.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	10	3.46	1.49	3.0
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	9	3.21	1.28	3.21
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	9	3.08	1.84	3.01
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	9	2.71	1.22	3.23
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	8	3.22	1.73	2.65
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	7	4.46	5.01	2.51
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	7	3.83	0.96	3.58
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	7	3.73	2.54	2.86
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	7	3.21	1.64	3.31
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	7	3.1	1.04	2.66
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	7	1.98	0.97	1.39
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	7	1.88	0.89	1.42
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	6	4.46	1.76	4.73
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	6	3.66	1.87	3.38
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	6	3.3	2.22	2.88
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	6	3.13	2.13	2.55
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	6	2.64	0.67	2.66
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	6	2.22	0.71	2.28
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	6	1.56	0.22	1.52
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	5	3.15	1.71	2.22
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	5	2.75	2.61	1.23
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	5	2.75	0.37	2.91
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	5	2.69	0.79	2.55
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	5	2.55	0.28	2.65
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	5	2.28	1.11	2.02
(1,6)	1:25:A:GLU:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	4	6.13	4.44	3.71
(1,164)	1:133:A:GLY:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	4	5.4	3.49	5.38
(1,78)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:VAL:N	4	4.14	2.38	3.37
(1,158)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	4	3.31	1.81	3.36
(1,145)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ASP:N	4	1.98	0.58	2.01
(1,130)	1:114:A:ASP:C	1:115:A:ILE:N	1:115:A:ILE:CA	1:115:A:ILE:C	4	1.55	0.32	1.6
(1,20)	1:33:A:ARG:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	3	5.83	1.04	6.23
(1,96)	1:87:A:HIS:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	3	5.24	2.25	5.33
(1,9)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:ALA:N	3	3.35	0.85	2.97
(1,122)	1:110:A:LEU:C	1:111:A:ASP:N	1:111:A:ASP:CA	1:111:A:ASP:C	3	3.18	0.94	2.56
(1,118)	1:107:A:GLY:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	3	2.39	0.99	2.47
(1,102)	1:90:A:GLY:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	3	1.7	0.25	1.67
(1,89)	1:85:A:PRO:N	1:85:A:PRO:CA	1:85:A:PRO:C	1:86:A:HIS:N	3	1.54	0.29	1.45
(1,77)	1:69:A:ASP:C	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	2	6.71	0.02	6.71
(1,125)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:ASP:N	2	4.28	1.31	4.28
(1,107)	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	1:95:A:ARG:N	2	3.81	2.37	3.81
(1,93)	1:87:A:HIS:N	1:87:A:HIS:CA	1:87:A:HIS:C	1:88:A:SER:N	2	3.52	0.04	3.52
(1,88)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	2	3.47	1.8	3.47
(1,128)	1:113:A:ARG:C	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	2	3.38	0.29	3.38
(1,160)	1:129:A:ALA:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	2	3.36	1.5	3.36
(1,150)	1:124:A:ASP:C	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	2	3.22	0.68	3.22
(1,137)	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	1:120:A:ASN:N	2	2.98	0.12	2.98
(1,48)	1:48:A:GLY:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	2	2.78	1.59	2.78
(1,149)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:ALA:N	2	2.08	0.24	2.08
(1,144)	1:121:A:PHE:C	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	2	2.02	0.12	2.02
(1,49)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:TYR:N	2	1.8	0.18	1.8

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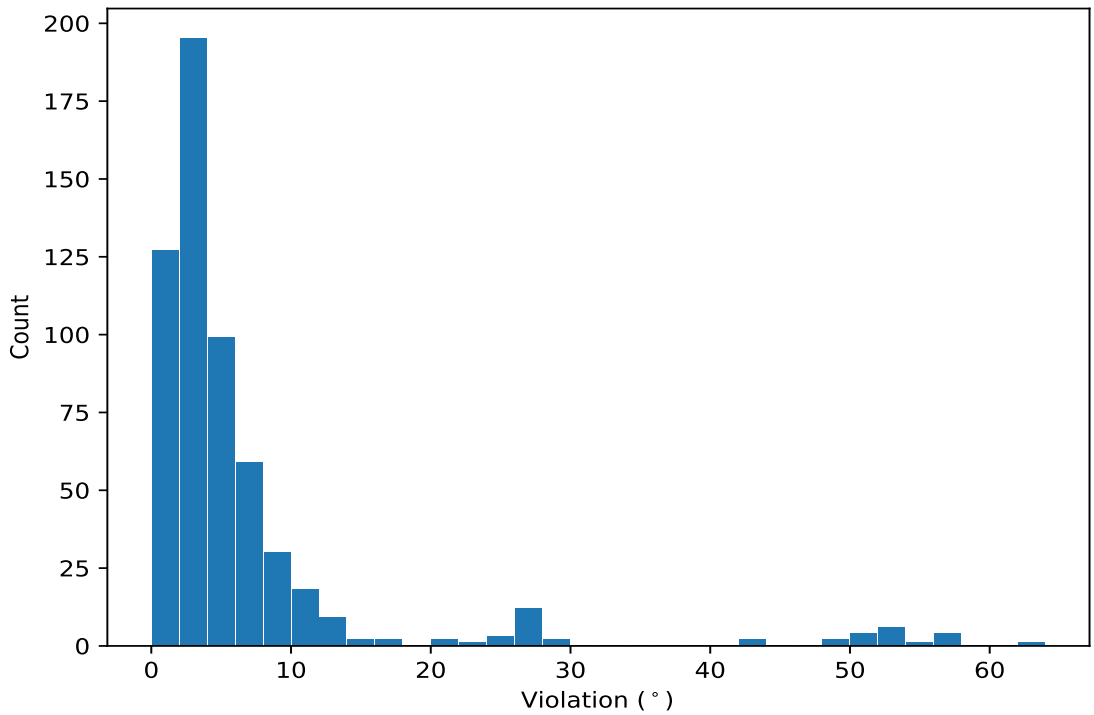
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,54)	1:51:A:TYR:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	2	1.52	0.38	1.52
(1,108)	1:93:A:ALA:C	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	2	1.41	0.22	1.41

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	10	62.5
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	11	57.89
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	2	57.46
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	13	57.36
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	17	56.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	7	54.01
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	9	53.68
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	12	53.54
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	19	53.26
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	16	53.22
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	14	52.53
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	5	52.19
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	18	51.55
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	15	51.41
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	20	50.78
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	1	50.68
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	8	49.67
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	3	48.97
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	6	42.63
(1,23)	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1:37:A:ILE:N	4	42.15
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	13	29.77
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	18	28.72
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	17	27.7
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	20	27.44
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	12	27.35
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	10	27.2
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	9	27.19
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	11	27.07
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	2	26.84
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	14	26.73
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	3	26.41
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	5	26.35
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1	26.09
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	8	26.02
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	7	25.83
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	19	25.36
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	15	24.87
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	16	23.27
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	6	21.57
(1,26)	1:36:A:PRO:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	4	21.33
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	17	16.79
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	3	16.51
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	16	15.04
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	4	14.65
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	11	13.99
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	9	13.81
(1,6)	1:25:A:GLU:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	14	13.81
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	1	13.7
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	7	13.67
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	6	13.46
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	2	13.42
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	6	12.75
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	13	12.39
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	3	11.85
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	18	11.8
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	10	11.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	1	11.29
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	3	11.29
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	11	11.19
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	16	11.16
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	9	11.08
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	4	11.02
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	14	10.9
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	16	10.81
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	15	10.63
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	18	10.58
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	5	10.16
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	2	10.12
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	14	10.11
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	17	10.08
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	12	10.02
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	10	9.93
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	7	9.81
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	5	9.66
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	20	9.63
(1,164)	1:133:A:GLY:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	20	9.48
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	13	9.18
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	3	9.15
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	11	9.14
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	19	9.12
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	15	9.11
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	19	9.07
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	3	9.0
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	3	8.95
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	1	8.78
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	10	8.78
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	19	8.76
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	15	8.65
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	7	8.53
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	17	8.53
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	7	8.52
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	1	8.49
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	13	8.27
(1,164)	1:133:A:GLY:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	19	8.19
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	2	8.14
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	3	8.13
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	20	8.12
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	13	8.09
(1,78)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:VAL:N	10	8.06
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	6	8.06
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	6	8.03
(1,96)	1:87:A:HIS:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	2	7.95
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	15	7.89
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	14	7.87
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	5	7.87
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	11	7.8
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1	7.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	16	7.79
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	19	7.64
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	18	7.62
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	17	7.61
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	2	7.52
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	5	7.41
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	13	7.27
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	1	7.26
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	9	7.16
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	14	7.13
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	9	7.12
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	4	7.09
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	5	7.07
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	4	7.03
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	10	7.01
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	15	6.98
(1,37)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	12	6.95
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	9	6.91
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	19	6.91
(1,20)	1:33:A:ARG:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	13	6.86
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	20	6.84
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	11	6.81
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	5	6.8
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	6	6.76
(1,77)	1:69:A:ASP:C	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	19	6.73
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	19	6.7
(1,77)	1:69:A:ASP:C	1:70:A:ALA:N	1:70:A:ALA:CA	1:70:A:ALA:C	9	6.69
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	14	6.65
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	2	6.6
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	14	6.59
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	3	6.57
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	5	6.52
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	12	6.44
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	18	6.39
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	3	6.37
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	10	6.29
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	20	6.29
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	8	6.27
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	13	6.25
(1,20)	1:33:A:ARG:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	19	6.23
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	15	6.19
(1,107)	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	1:95:A:ARG:N	20	6.18
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	11	6.18
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	5	6.11
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	18	6.11
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	12	6.11
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	5	6.08
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	4	6.07
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	5	6.06
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	20	6.04
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	10	6.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	5	6.02
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	19	6.01
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	17	5.98
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	13	5.94
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	20	5.93
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	10	5.91
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	8	5.89
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	9	5.89
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	14	5.87
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	12	5.85
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	17	5.81
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	6	5.81
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	8	5.8
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	17	5.8
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	3	5.76
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	7	5.74
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	13	5.73
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	8	5.73
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	19	5.69
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	10	5.67
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	18	5.64
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	11	5.62
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	3	5.61
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	4	5.61
(1,125)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:ASP:N	9	5.6
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	11	5.55
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	9	5.5
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	10	5.46
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	3	5.41
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	15	5.37
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	8	5.35
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	18	5.34
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	8	5.34
(1,96)	1:87:A:HIS:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	10	5.33
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	2	5.3
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	20	5.29
(1,88)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	10	5.27
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	12	5.25
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	9	5.24
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	14	5.24
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	15	5.23
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	11	5.23
(1,158)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	18	5.22
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	17	5.22
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	9	5.12
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	19	5.11
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	6	5.08
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	14	5.02
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	16	5.02
(1,158)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	7	5.01
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	11	4.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	17	4.94
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	19	4.94
(1,160)	1:129:A:ALA:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	18	4.86
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	11	4.86
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	20	4.83
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	8	4.77
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	12	4.76
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	13	4.69
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	16	4.68
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	3	4.66
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	16	4.66
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	2	4.66
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	3	4.64
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	18	4.63
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	5	4.63
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	12	4.61
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	20	4.6
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	10	4.59
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	13	4.59
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	2	4.58
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	7	4.57
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	14	4.56
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	15	4.55
(1,9)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:ALA:N	8	4.53
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	16	4.52
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	8	4.51
(1,122)	1:110:A:LEU:C	1:111:A:ASP:N	1:111:A:ASP:CA	1:111:A:ASP:C	1	4.5
(1,162)	1:132:A:ALA:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	8	4.49
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	18	4.44
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	7	4.42
(1,20)	1:33:A:ARG:C	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	5	4.41
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	5	4.4
(1,48)	1:48:A:GLY:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	6	4.38
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	9	4.38
(1,84)	1:81:A:VAL:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	6	4.29
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	4	4.27
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	16	4.27
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	10	4.26
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	2	4.25
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	17	4.24
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	15	4.17
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	20	4.16
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	12	4.14
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	14	4.12
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	9	4.1
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	9	4.06
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	6	4.05
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	14	4.02
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	16	4.01
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	13	4.0
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	8	3.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	4	3.94
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	19	3.94
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	19	3.94
(1,150)	1:124:A:ASP:C	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	12	3.91
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	10	3.89
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	7	3.89
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	13	3.88
(1,78)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:VAL:N	17	3.88
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	13	3.86
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	1	3.85
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	20	3.85
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	19	3.84
(1,91)	1:86:A:HIS:N	1:86:A:HIS:CA	1:86:A:HIS:C	1:87:A:HIS:N	11	3.83
(1,6)	1:25:A:GLU:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	20	3.82
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	7	3.8
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	11	3.78
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	11	3.77
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	10	3.77
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	15	3.76
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	20	3.75
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	4	3.7
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	9	3.7
(1,128)	1:113:A:ARG:C	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	10	3.67
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	15	3.67
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	15	3.66
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	9	3.66
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	13	3.65
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	18	3.62
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	12	3.61
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	11	3.61
(1,6)	1:25:A:GLU:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	13	3.6
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	5	3.59
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	20	3.58
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	14	3.57
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1	3.57
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	17	3.56
(1,118)	1:107:A:GLY:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	15	3.56
(1,93)	1:87:A:HIS:N	1:87:A:HIS:CA	1:87:A:HIS:C	1:88:A:SER:N	10	3.56
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	1	3.56
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	12	3.56
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	15	3.55
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	8	3.54
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	2	3.53
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	16	3.53
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	14	3.51
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	15	3.5
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	12	3.49
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	7	3.49
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	19	3.47
(1,93)	1:87:A:HIS:N	1:87:A:HIS:CA	1:87:A:HIS:C	1:88:A:SER:N	2	3.47
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	8	3.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	4	3.44
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	2	3.43
(1,156)	1:127:A:GLN:C	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	16	3.39
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	13	3.38
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	3	3.37
(1,27)	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	1:39:A:PRO:N	20	3.36
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	2	3.34
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	1	3.34
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	15	3.34
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	3	3.33
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	10	3.31
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	20	3.31
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	18	3.31
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	1	3.3
(1,6)	1:25:A:GLU:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	4	3.3
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	8	3.28
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	17	3.25
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	18	3.24
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	8	3.23
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	2	3.21
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	18	3.21
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	15	3.21
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	9	3.2
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	5	3.18
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	4	3.15
(1,137)	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	1:120:A:ASN:N	13	3.1
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	14	3.1
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	9	3.1
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	4	3.09
(1,128)	1:113:A:ARG:C	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	4	3.08
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	12	3.08
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	17	3.06
(1,153)	1:127:A:GLN:N	1:127:A:GLN:CA	1:127:A:GLN:C	1:128:A:GLY:N	17	3.05
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	2	3.05
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	8	3.05
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	7	3.05
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	2	3.04
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	18	3.04
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	17	3.04
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	5	3.01
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	20	2.99
(1,125)	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1:114:A:ASP:N	4	2.97
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	10	2.97
(1,9)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:ALA:N	18	2.97
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	9	2.96
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	20	2.95
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	2	2.94
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	15	2.94
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	7	2.93
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	2	2.93
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	13	2.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	14	2.91
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	18	2.91
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	10	2.88
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	9	2.87
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	4	2.87
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	6	2.87
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	8	2.87
(1,139)	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	1:121:A:PHE:N	19	2.86
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	12	2.86
(1,78)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:VAL:N	6	2.86
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	6	2.86
(1,154)	1:126:A:ALA:C	1:127:A:GLN:N	1:127:A:GLN:CA	1:127:A:GLN:C	16	2.85
(1,137)	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	1:120:A:ASN:N	11	2.85
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	7	2.84
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	4	2.83
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	7	2.8
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	8	2.78
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	12	2.75
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	5	2.75
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	3	2.73
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	6	2.69
(1,145)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ASP:N	11	2.68
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	6	2.66
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	8	2.66
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	18	2.66
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	10	2.65
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	2	2.65
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	14	2.6
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	17	2.6
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1	2.59
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	11	2.59
(1,164)	1:133:A:GLY:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	14	2.58
(1,122)	1:110:A:LEU:C	1:111:A:ASP:N	1:111:A:ASP:CA	1:111:A:ASP:C	10	2.56
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	12	2.56
(1,9)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:ALA:N	11	2.56
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	10	2.55
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	15	2.55
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	16	2.55
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	5	2.55
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	17	2.55
(1,150)	1:124:A:ASP:C	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	15	2.54
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	7	2.54
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	12	2.53
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	7	2.53
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1	2.53
(1,17)	1:32:A:HIS:N	1:32:A:HIS:CA	1:32:A:HIS:C	1:33:A:ARG:N	8	2.53
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	6	2.52
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	4	2.51
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	17	2.49
(1,122)	1:110:A:LEU:C	1:111:A:ASP:N	1:111:A:ASP:CA	1:111:A:ASP:C	15	2.47
(1,118)	1:107:A:GLY:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	6	2.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,56)	1:52:A:ALA:C	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	4	2.47
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	8	2.46
(1,81)	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1:82:A:GLU:N	3	2.46
(1,96)	1:87:A:HIS:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	9	2.43
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	16	2.42
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	8	2.41
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	16	2.4
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	6	2.37
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	19	2.37
(1,145)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ASP:N	4	2.36
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	14	2.34
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	10	2.34
(1,149)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:ALA:N	13	2.32
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	20	2.32
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	9	2.32
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	19	2.3
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	9	2.28
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	9	2.24
(1,159)	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	1:131:A:LEU:N	6	2.22
(1,155)	1:128:A:GLY:N	1:128:A:GLY:CA	1:128:A:GLY:C	1:129:A:ALA:N	9	2.22
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	16	2.22
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	11	2.21
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	10	2.18
(1,144)	1:121:A:PHE:C	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	5	2.15
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	11	2.14
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	13	2.13
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	17	2.13
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	14	2.11
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1	2.11
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	10	2.09
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	11	2.09
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	4	2.08
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	17	2.08
(1,115)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:GLY:N	14	2.07
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	20	2.06
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	11	2.05
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	5	2.02
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	3	2.02
(1,102)	1:90:A:GLY:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	11	2.01
(1,71)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	18	2.0
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	2	2.0
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	4	1.98
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	13	1.98
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	1	1.98
(1,49)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:TYR:N	12	1.98
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	20	1.97
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	6	1.96
(1,61)	1:56:A:VAL:N	1:56:A:VAL:CA	1:56:A:VAL:C	1:57:A:ARG:N	7	1.94
(1,89)	1:85:A:PRO:N	1:85:A:PRO:CA	1:85:A:PRO:C	1:86:A:HIS:N	4	1.93
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	7	1.92
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	12	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:114:A:ASP:C	1:115:A:ILE:N	1:115:A:ILE:CA	1:115:A:ILE:C	9	1.91
(1,163)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:ASN:N	18	1.9
(1,144)	1:121:A:PHE:C	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	2	1.9
(1,54)	1:51:A:TYR:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	14	1.9
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	14	1.89
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	5	1.88
(1,161)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	7	1.87
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	9	1.87
(1,160)	1:129:A:ALA:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	7	1.86
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	7	1.86
(1,149)	1:125:A:ARG:N	1:125:A:ARG:CA	1:125:A:ARG:C	1:126:A:ALA:N	19	1.84
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	9	1.84
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	10	1.84
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	2	1.83
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	10	1.8
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1	1.78
(1,130)	1:114:A:ASP:C	1:115:A:ILE:N	1:115:A:ILE:CA	1:115:A:ILE:C	16	1.77
(1,45)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:VAL:N	17	1.77
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	3	1.77
(1,78)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:VAL:N	14	1.76
(1,123)	1:112:A:GLU:N	1:112:A:GLU:CA	1:112:A:GLU:C	1:113:A:ARG:N	4	1.75
(1,158)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	15	1.7
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	12	1.7
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	8	1.7
(1,145)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ASP:N	20	1.67
(1,134)	1:116:A:TRP:C	1:117:A:ASP:N	1:117:A:ASP:CA	1:117:A:ASP:C	8	1.67
(1,102)	1:90:A:GLY:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	13	1.67
(1,88)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	17	1.67
(1,98)	1:88:A:SER:C	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	9	1.66
(1,4)	1:24:A:TRP:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	15	1.66
(1,65)	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	1:62:A:THR:N	4	1.65
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	8	1.64
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	5	1.64
(1,12)	1:28:A:GLU:C	1:29:A:ALA:N	1:29:A:ALA:CA	1:29:A:ALA:C	19	1.64
(1,108)	1:93:A:ALA:C	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	8	1.63
(1,49)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:TYR:N	1	1.63
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	3	1.61
(1,167)	1:135:A:ASN:C	1:136:A:GLY:N	1:136:A:GLY:CA	1:136:A:GLY:C	19	1.6
(1,59)	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	1:56:A:VAL:N	13	1.57
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	2	1.57
(1,29)	1:39:A:PRO:N	1:39:A:PRO:CA	1:39:A:PRO:C	1:40:A:ASP:N	16	1.57
(1,66)	1:60:A:GLY:C	1:61:A:GLU:N	1:61:A:GLU:CA	1:61:A:GLU:C	11	1.55
(1,34)	1:41:A:ALA:C	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	11	1.55
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	16	1.54
(1,39)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:GLN:N	20	1.54
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	16	1.54
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	9	1.52
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	16	1.51
(1,3)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:VAL:N	3	1.51
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	17	1.5
(1,58)	1:53:A:GLU:C	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	11	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	1	1.5
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	11	1.49
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	14	1.49
(1,1)	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	1:25:A:GLU:N	1	1.49
(1,2)	1:23:A:GLY:C	1:24:A:TRP:N	1:24:A:TRP:CA	1:24:A:TRP:C	12	1.48
(1,157)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ALA:N	15	1.47
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	12	1.47
(1,38)	1:43:A:SER:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	4	1.46
(1,97)	1:89:A:ASP:N	1:89:A:ASP:CA	1:89:A:ASP:C	1:90:A:GLY:N	19	1.45
(1,89)	1:85:A:PRO:N	1:85:A:PRO:CA	1:85:A:PRO:C	1:86:A:HIS:N	3	1.45
(1,53)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:GLU:N	16	1.45
(1,130)	1:114:A:ASP:C	1:115:A:ILE:N	1:115:A:ILE:CA	1:115:A:ILE:C	12	1.44
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	14	1.44
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	16	1.44
(1,107)	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	1:95:A:ARG:N	6	1.44
(1,126)	1:112:A:GLU:C	1:113:A:ARG:N	1:113:A:ARG:CA	1:113:A:ARG:C	1	1.43
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	19	1.42
(1,83)	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	1:83:A:HIS:N	3	1.42
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	8	1.42
(1,102)	1:90:A:GLY:C	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	17	1.41
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	18	1.41
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	19	1.39
(1,117)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ALA:N	20	1.38
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	5	1.38
(1,164)	1:133:A:GLY:C	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	2	1.37
(1,69)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:GLY:N	19	1.37
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	8	1.37
(1,60)	1:54:A:HIS:C	1:55:A:CYS:N	1:55:A:CYS:CA	1:55:A:CYS:C	15	1.36
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	12	1.35
(1,158)	1:128:A:GLY:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	10	1.33
(1,151)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:GLN:N	8	1.32
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	1	1.32
(1,136)	1:117:A:ASP:C	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	3	1.32
(1,110)	1:94:A:TYR:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	11	1.28
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	10	1.26
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	19	1.25
(1,40)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	11	1.24
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	7	1.24
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	6	1.23
(1,89)	1:85:A:PRO:N	1:85:A:PRO:CA	1:85:A:PRO:C	1:86:A:HIS:N	16	1.23
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	18	1.23
(1,32)	1:40:A:ASP:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	17	1.22
(1,166)	1:134:A:THR:C	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	8	1.2
(1,145)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ASP:N	10	1.2
(1,36)	1:42:A:ARG:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	4	1.2
(1,108)	1:93:A:ALA:C	1:94:A:TYR:N	1:94:A:TYR:CA	1:94:A:TYR:C	14	1.19
(1,48)	1:48:A:GLY:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	14	1.19
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	11	1.17
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	5	1.16
(1,147)	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	1:125:A:ARG:N	9	1.15
(1,113)	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	1:98:A:ILE:N	17	1.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:51:A:TYR:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	9	1.15
(1,118)	1:107:A:GLY:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	7	1.13
(1,55)	1:53:A:GLU:N	1:53:A:GLU:CA	1:53:A:GLU:C	1:54:A:HIS:N	2	1.13
(1,109)	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	1:96:A:VAL:N	6	1.12
(1,7)	1:27:A:PRO:N	1:27:A:PRO:CA	1:27:A:PRO:C	1:28:A:GLU:N	12	1.11
(1,70)	1:63:A:LEU:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	19	1.1
(1,135)	1:118:A:LEU:N	1:118:A:LEU:CA	1:118:A:LEU:C	1:119:A:VAL:N	8	1.09
(1,130)	1:114:A:ASP:C	1:115:A:ILE:N	1:115:A:ILE:CA	1:115:A:ILE:C	18	1.07
(1,72)	1:65:A:GLY:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	15	1.07
(1,31)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:ARG:N	4	1.06
(1,24)	1:35:A:ASN:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	3	1.06
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	1	1.05
(1,112)	1:95:A:ARG:C	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	17	1.03
(1,143)	1:122:A:MET:N	1:122:A:MET:CA	1:122:A:MET:C	1:123:A:ARG:N	20	1.01
(1,101)	1:91:A:ASP:N	1:91:A:ASP:CA	1:91:A:ASP:C	1:92:A:LEU:N	2	1.01